

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
 Data File : BF126111.D
 Acq On : 10 Nov 2021 17:09
 Operator : JU/CG
 Sample : M4595-08
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CMC-ICS-003-004

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	4	13	19	rVB	1746381	2192997	42.98%	4.620%
2	2.269	26	31	40	rBV2	60831	92108	1.81%	0.194%
3	2.499	59	70	79	rVB	105701	244109	4.78%	0.514%
4	4.451	397	402	409	rVB	1110593	1168568	22.90%	2.462%
5	5.081	500	509	512	rBV	2440136	3110568	60.97%	6.553%
6	5.475	572	576	579	rBV	2785711	2384936	46.75%	5.024%
7	6.487	742	748	751	rBV	4287127	4358543	85.43%	9.182%
8	6.851	807	810	814	rBV	1271151	1057333	20.72%	2.227%
9	7.416	898	906	909	rBV	3273917	2927848	57.39%	6.168%
10	8.039	1008	1012	1021	rBV	633861	709018	13.90%	1.494%
11	8.134	1023	1028	1032	rBV	1508481	1251141	24.52%	2.636%
12	9.210	1206	1211	1214	rBV	5981067	5101909	100.00%	10.748%
13	9.292	1221	1225	1227	rBV	67829	64186	1.26%	0.135%
14	9.328	1227	1231	1234	rVB	163628	140701	2.76%	0.296%
15	9.886	1319	1326	1330	rBV	1465189	1341869	26.30%	2.827%
16	10.322	1397	1400	1402	rVB	120957	92843	1.82%	0.196%
17	10.433	1415	1419	1425	rBV2	68554	83309	1.63%	0.175%
18	10.539	1432	1437	1440	rBV4	96277	154863	3.04%	0.326%
19	10.669	1455	1459	1464	rBV2	295619	335631	6.58%	0.707%
20	10.763	1472	1475	1478	rBV	97758	116912	2.29%	0.246%
21	10.792	1478	1480	1482	rBV	167743	169079	3.31%	0.356%
22	10.945	1499	1506	1509	rBV	173097	250065	4.90%	0.527%
23	10.986	1510	1513	1517	rBV	179494	252888	4.96%	0.533%
24	11.080	1526	1529	1531	rBV2	80529	71236	1.40%	0.150%
25	11.116	1533	1535	1537	rBV	81745	84595	1.66%	0.178%
26	11.239	1553	1556	1558	rBV2	232784	241704	4.74%	0.509%
27	11.275	1558	1562	1564	rVV2	286628	380123	7.45%	0.801%
28	11.374	1575	1579	1581	rBV	1192517	1158556	22.71%	2.441%
29	11.398	1581	1583	1585	rVV	497708	387164	7.59%	0.816%
30	11.422	1585	1587	1589	rVV2	163313	177330	3.48%	0.374%
31	11.486	1596	1598	1601	rVB3	139681	131886	2.59%	0.278%
32	11.516	1601	1603	1607	rBV3	151680	198522	3.89%	0.418%
33	11.557	1607	1610	1613	rBV2	252203	330061	6.47%	0.695%
34	11.680	1627	1631	1635	rBV2	330770	642432	12.59%	1.353%
35	11.833	1654	1657	1659	rBV	343880	348999	6.84%	0.735%
36	11.874	1662	1664	1666	rVV	231119	169260	3.32%	0.357%

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37	11.904	1666	1669	1672	rVB	330221	284836	5.58%	0.600%
38	11.969	1677	1680	1681	rBV	304724	309292	6.06%	0.652%
39	12.080	1697	1699	1702	rBV	409341	465614	9.13%	0.981%
40	12.192	1716	1718	1721	rBV2	228861	241721	4.74%	0.509%
41	12.233	1722	1725	1727	rBV2	258457	349603	6.85%	0.736%
42	12.357	1743	1746	1751	rBV2	576576	772034	15.13%	1.626%
43	12.398	1751	1753	1756	rVB2	356012	325364	6.38%	0.685%
44	12.474	1763	1766	1768	rBV	437787	522123	10.23%	1.100%
45	12.586	1782	1785	1787	rBV	895699	788062	15.45%	1.660%
46	12.610	1787	1789	1792	rVV	224967	263231	5.16%	0.555%
47	12.816	1821	1824	1826	rVB	684283	575928	11.29%	1.213%
48	12.839	1826	1828	1830	rBV	394708	316305	6.20%	0.666%
49	12.869	1831	1833	1840	rVB2	431496	581478	11.40%	1.225%
50	12.963	1845	1849	1852	rBV	5207423	4818495	94.44%	10.151%
51	13.863	2000	2002	2013	rVB2	476053	858854	16.83%	1.809%
52	14.016	2023	2028	2030	rBV2	1114938	1365966	26.77%	2.878%
53	14.039	2030	2032	2035	rVB	343052	259467	5.09%	0.547%
54	14.663	2135	2138	2142	rBV	291026	271599	5.32%	0.572%
55	14.868	2171	2173	2176	rVB	215942	200366	3.93%	0.422%
56	15.051	2202	2204	2212	rVB	259455	462634	9.07%	0.975%
57	15.415	2263	2266	2269	rVB	152428	164408	3.22%	0.346%
58	15.480	2273	2277	2280	rBV	648283	732580	14.36%	1.543%
59	15.962	2355	2359	2367	rVB2	243231	409872	8.03%	0.863%
60	16.192	2395	2398	2401	rBV4	127006	206473	4.05%	0.435%

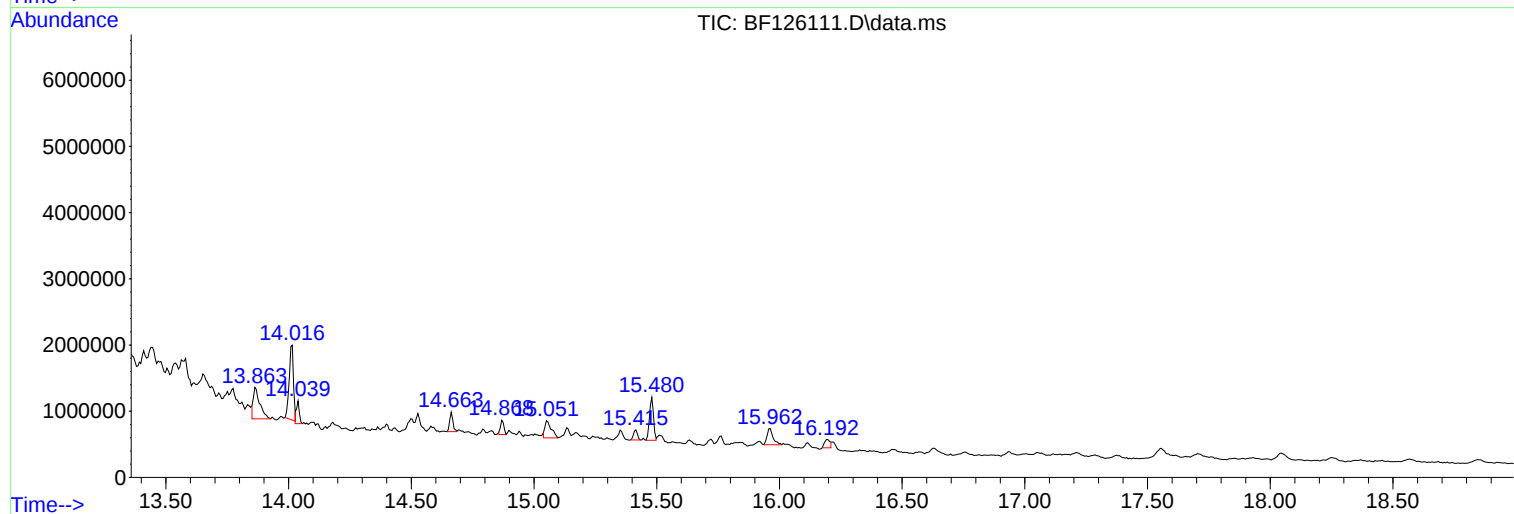
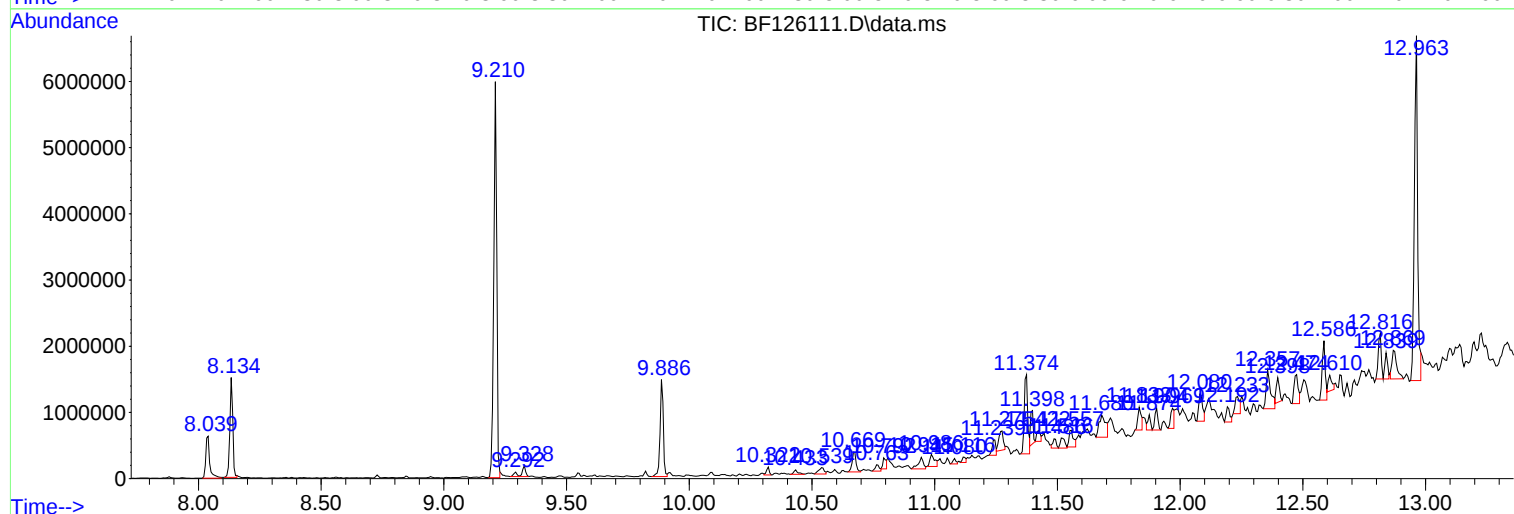
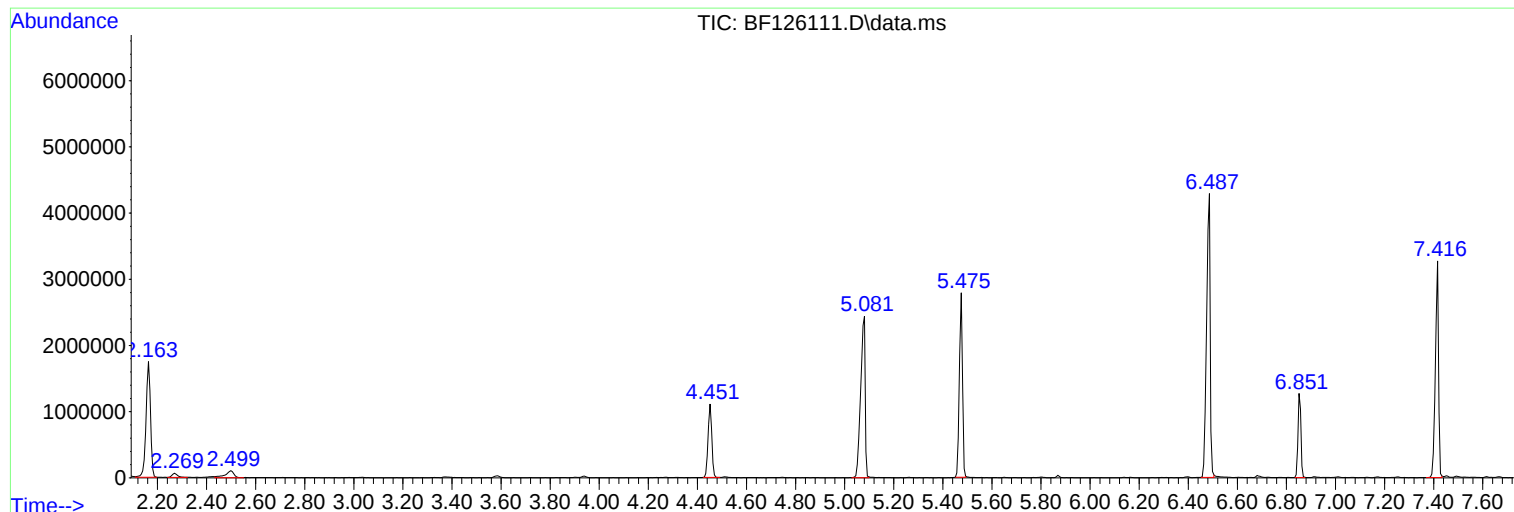
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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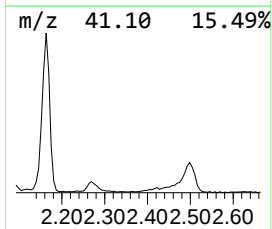
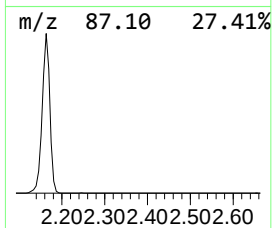
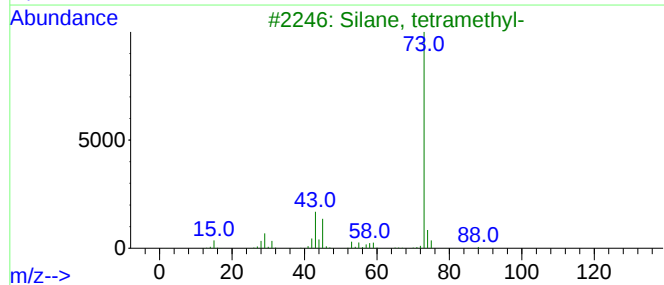
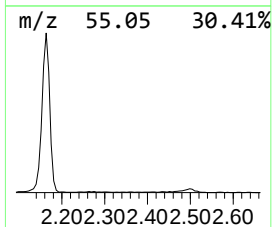
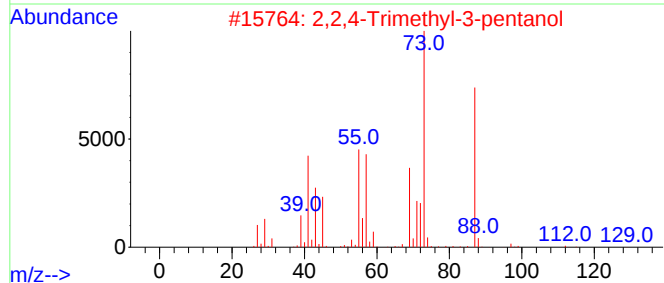
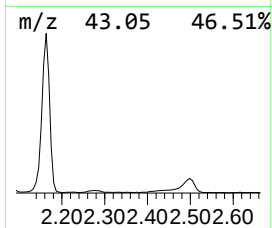
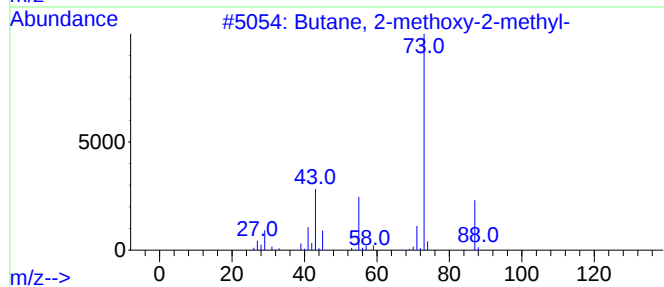
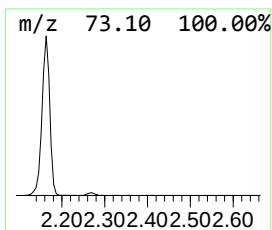
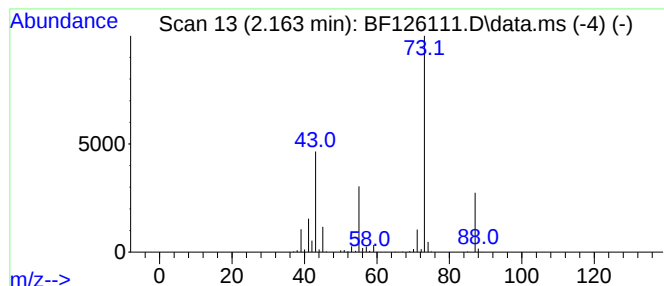
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	41.48 ng	2193000	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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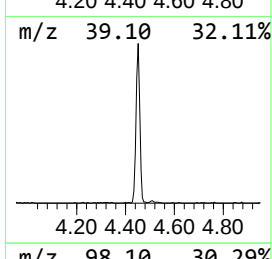
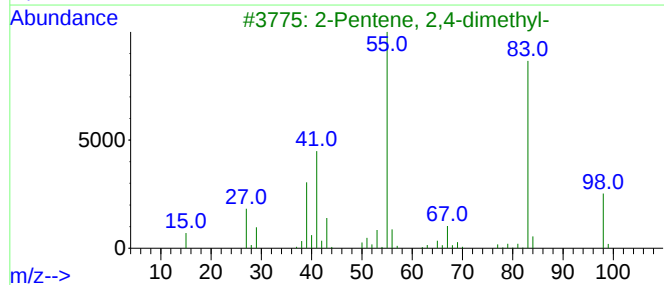
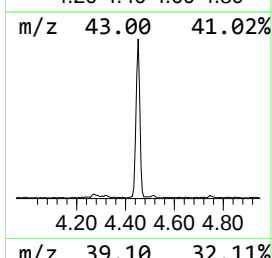
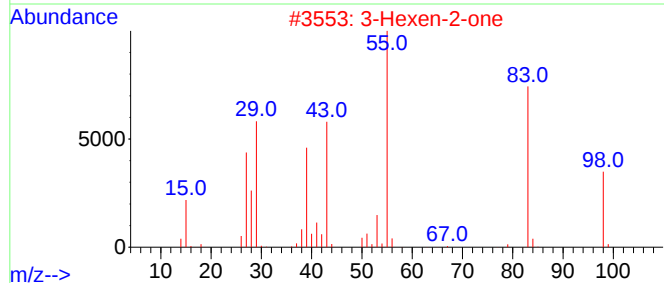
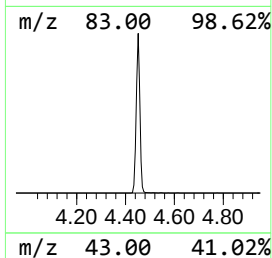
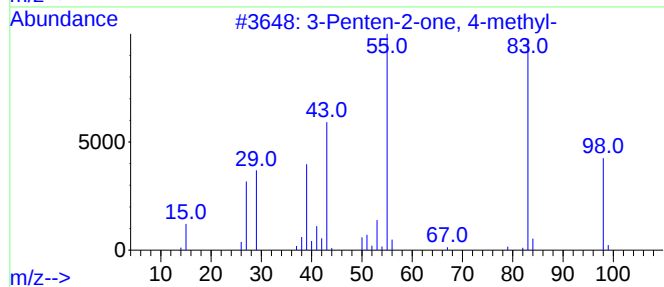
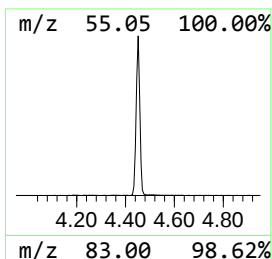
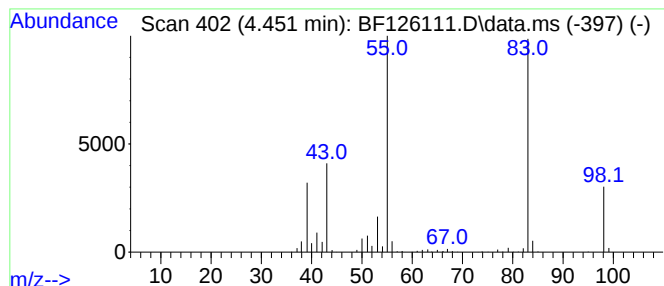
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.451	22.10 ng	1168570	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	91
2	3-Hexen-2-one			98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-			98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (E)-			98	C7H14	004914-92-5	86
5	2-Pentene, 4,4-dimethyl-, (E)-			98	C7H14	000690-08-4	78



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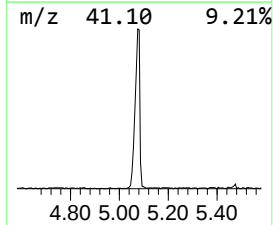
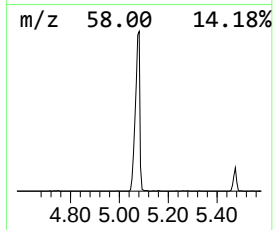
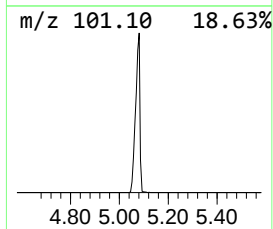
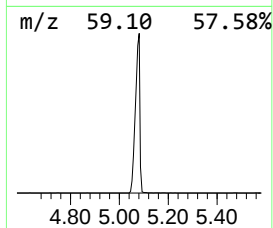
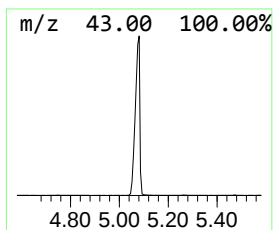
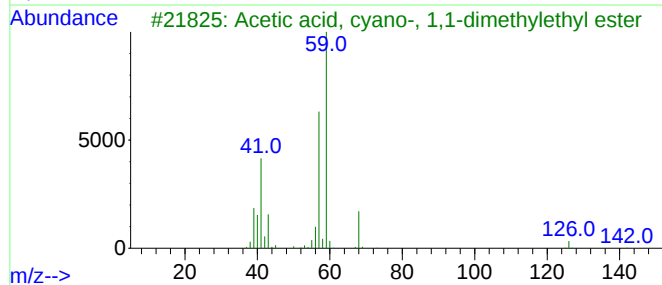
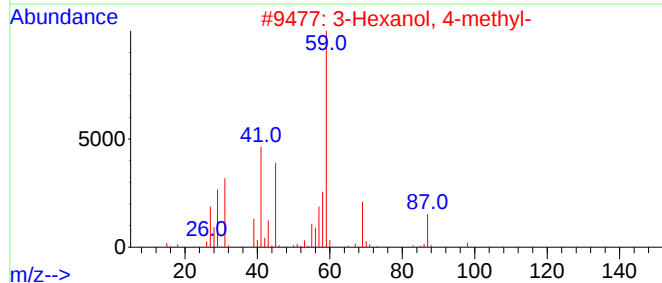
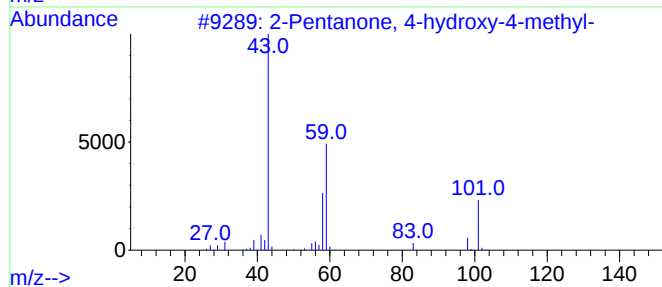
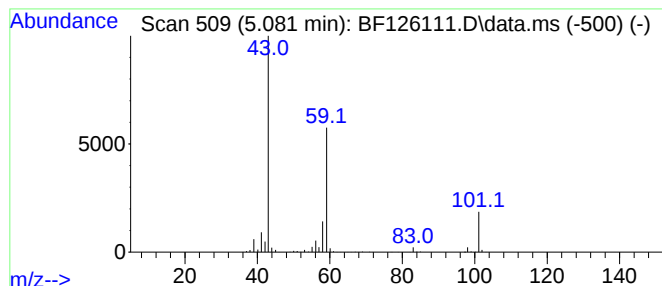
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.081	58.84 ng	3110570	1,4-Dichlorobenzene-d4			6.851
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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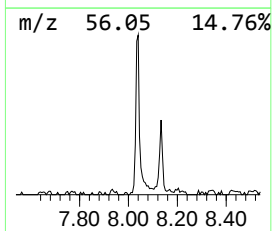
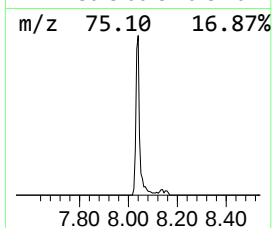
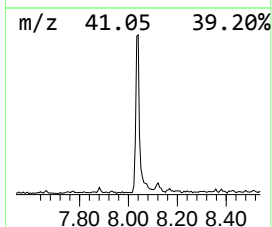
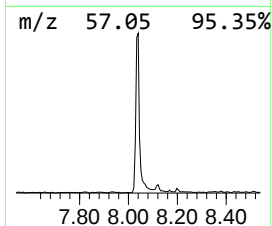
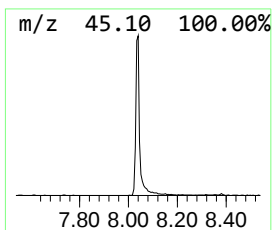
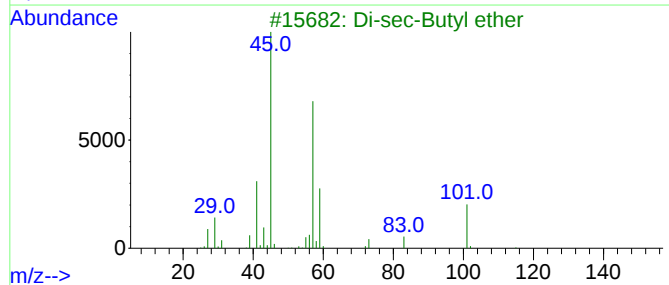
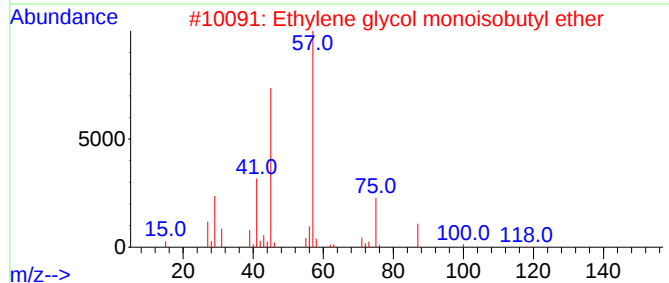
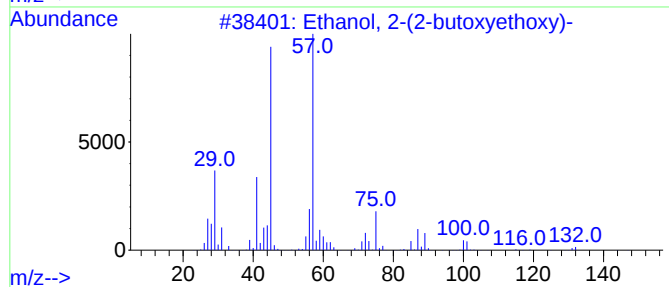
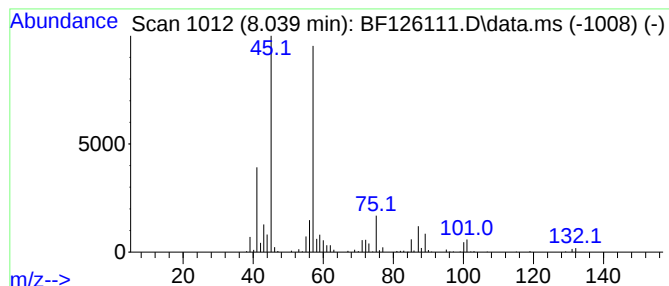
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	11.33 ng	709018	Naphthalene-d8	8.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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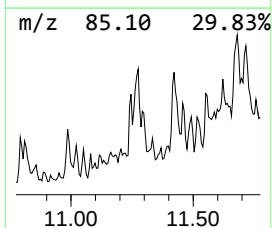
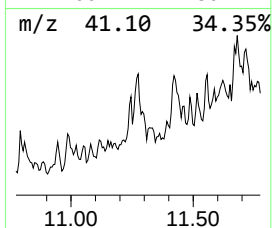
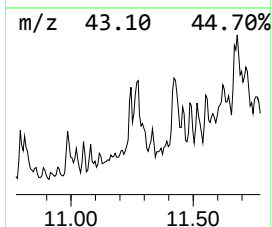
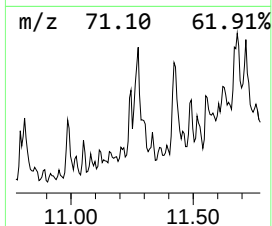
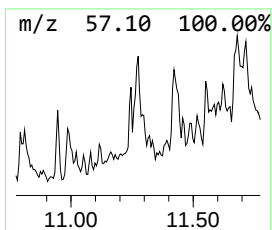
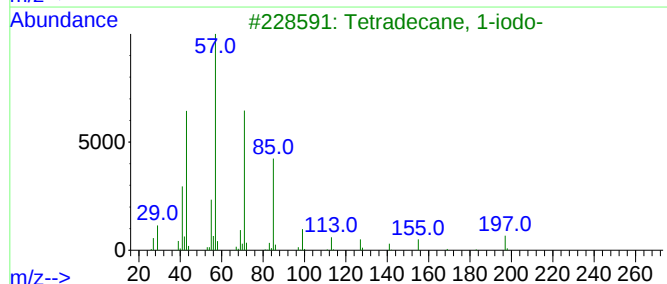
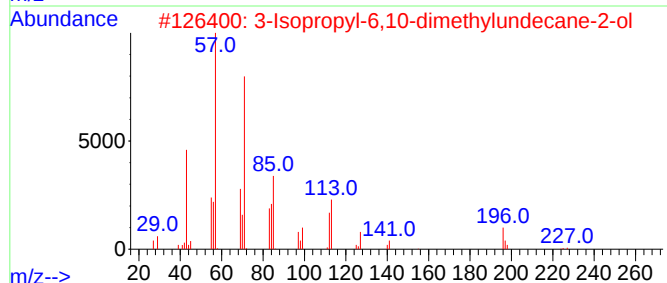
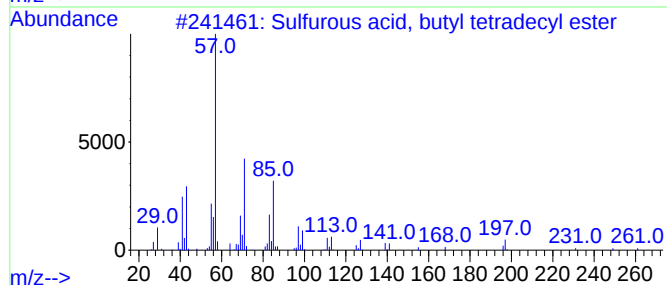
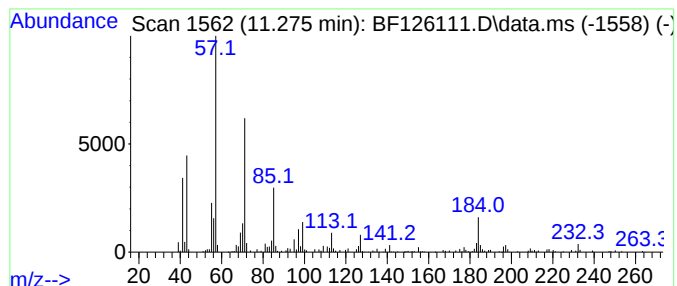
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, butyl tetra... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.275	6.56 ng	380123	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	72
2			3-Isopropyl-6,10-dimethylundecan...	242	C16H34O	1000432-47-1	64
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
4			Heptacosane	380	C27H56	000593-49-7	64
5			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
Acq On : 10 Nov 2021 17:09
Operator : JU/CG
Sample : M4595-08
Misc :
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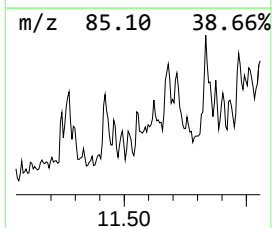
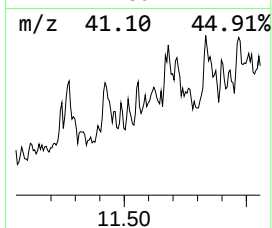
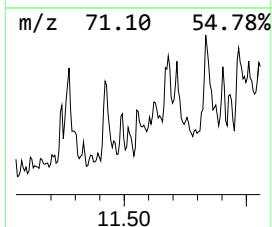
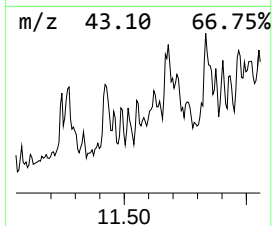
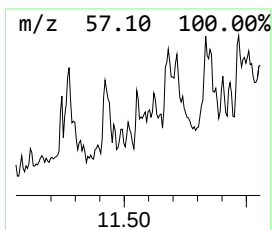
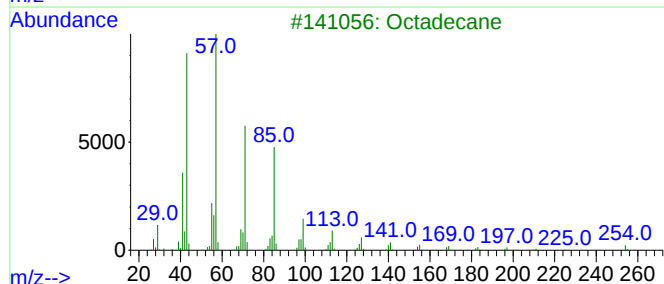
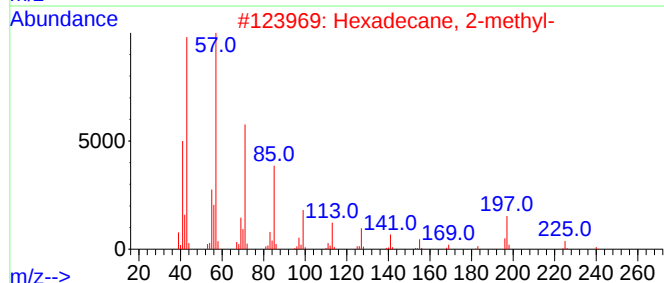
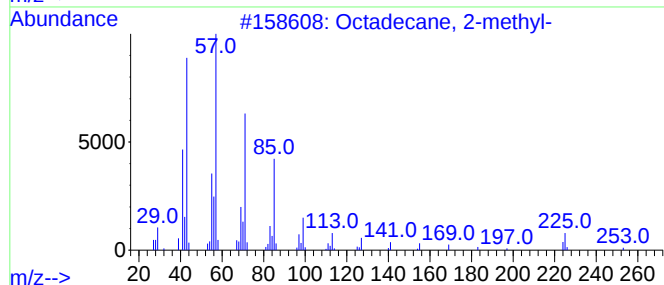
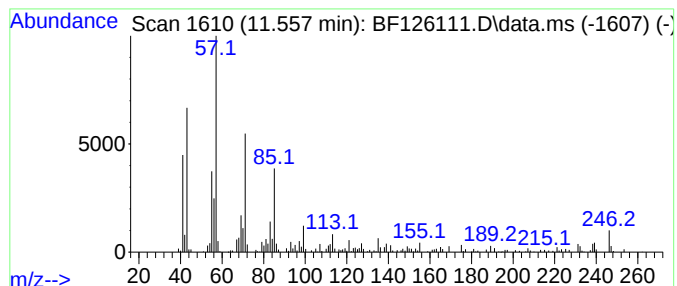
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ClientSampleId :
CMC-ICS-003-004

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane, 2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.557	5.70 ng	330061	Phenanthrene-d10	11.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	74
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	74
3	Octadecane	254	C18H38	000593-45-3	68
4	Heneicosane	296	C21H44	000629-94-7	68
5	Octacosane	394	C28H58	000630-02-4	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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Acq On : 10 Nov 2021 17:09
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Sample : M4595-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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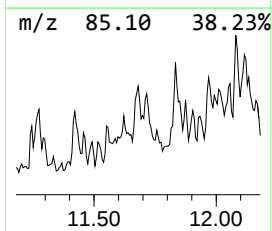
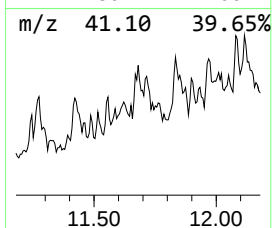
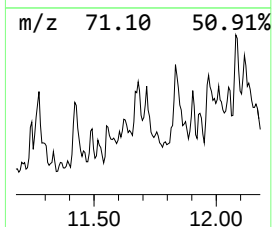
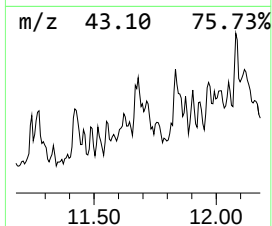
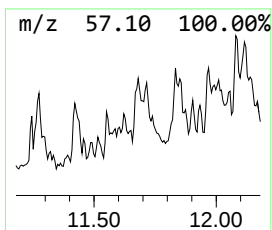
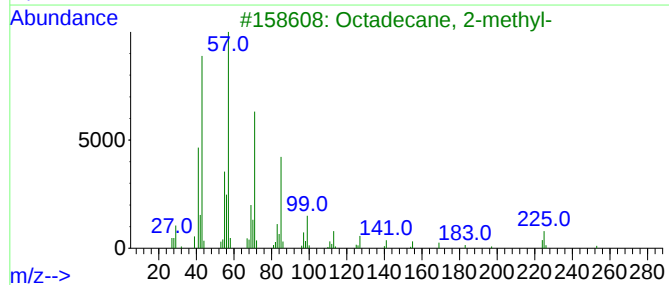
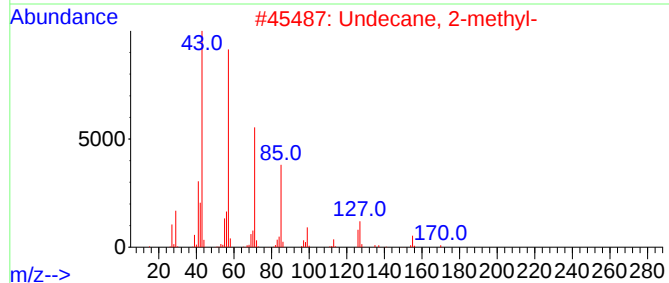
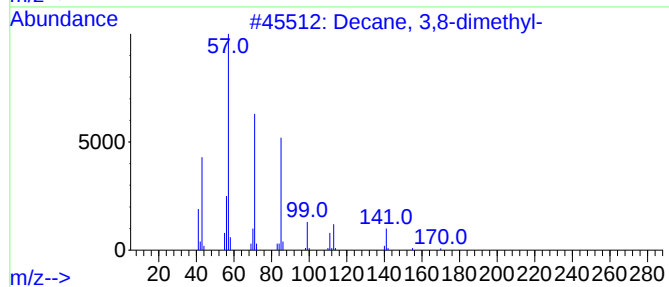
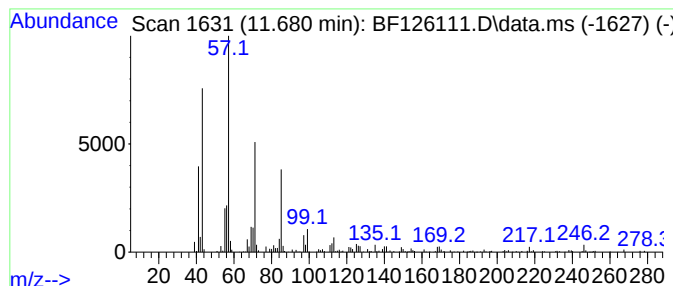
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Undecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.680	11.09 ng	642432	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
2			Undecane, 2-methyl-	170	C12H26	007045-71-8	86
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
4			Hexadecane	226	C16H34	000544-76-3	86
5			Undecane, 5-methyl-	170	C12H26	001632-70-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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Acq On : 10 Nov 2021 17:09
Operator : JU/CG
Sample : M4595-08
Misc :
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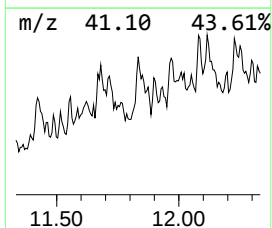
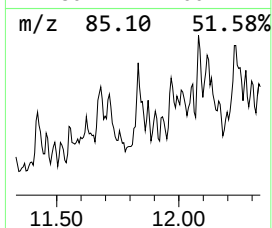
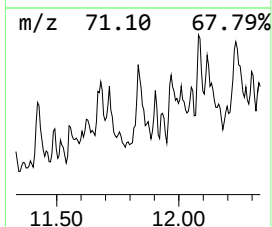
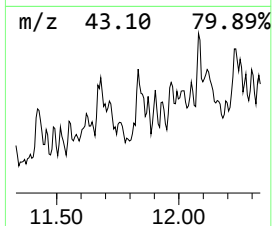
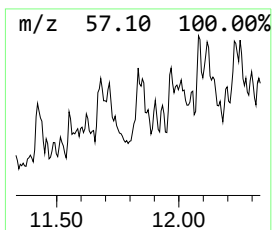
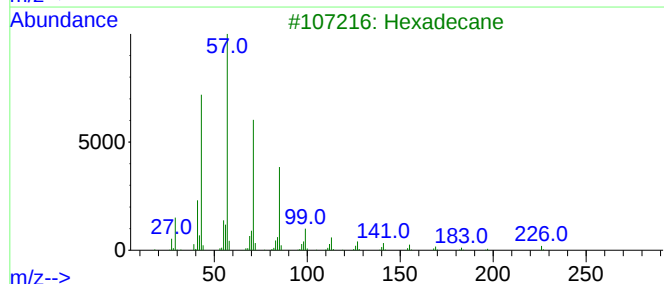
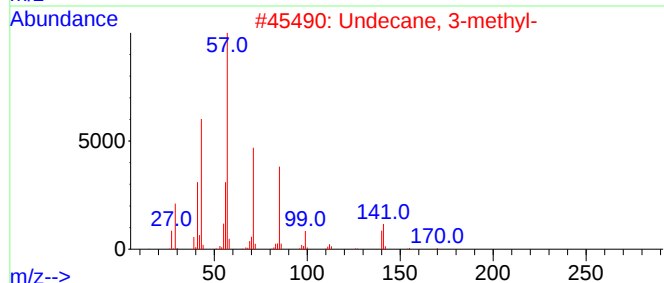
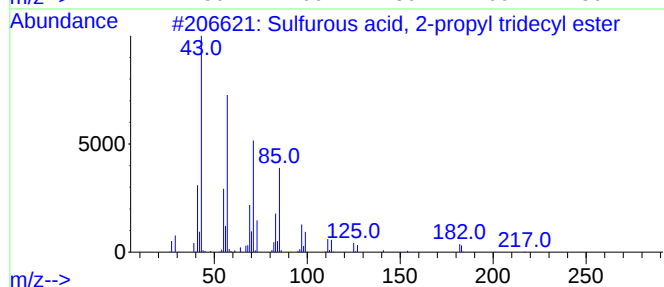
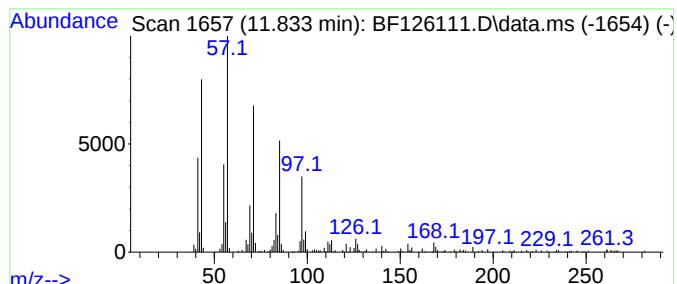
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Sulfurous acid, 2-propyl tr... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.833	6.02 ng	348999	Phenanthrene-d10		11.374	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...		306	C16H34O3S	1000309-12-4	72
2	Undecane, 3-methyl-		170	C12H26	001002-43-3	64
3	Hexadecane		226	C16H34	000544-76-3	64
4	Tetradecane		198	C14H30	000629-59-4	64
5	Dodecane, 4-methyl-		184	C13H28	006117-97-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
Acq On : 10 Nov 2021 17:09
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Instrument :
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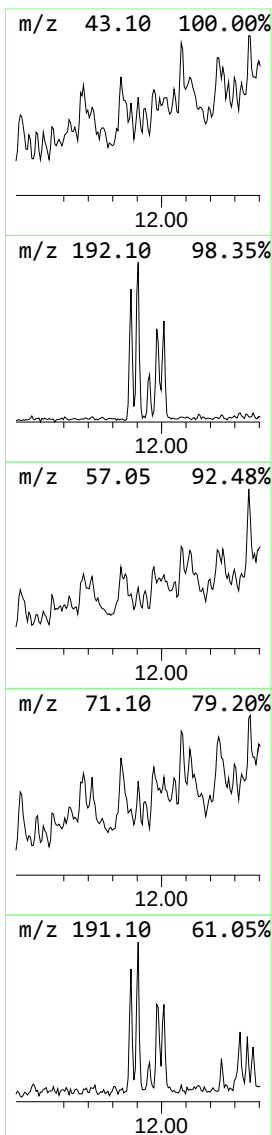
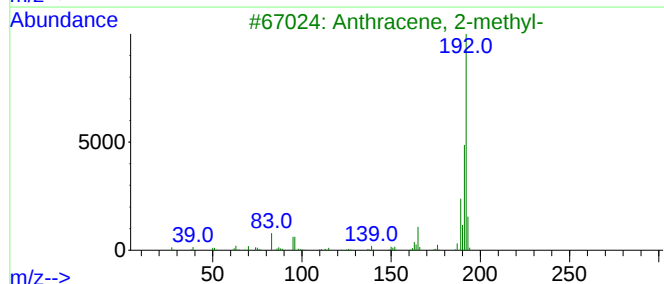
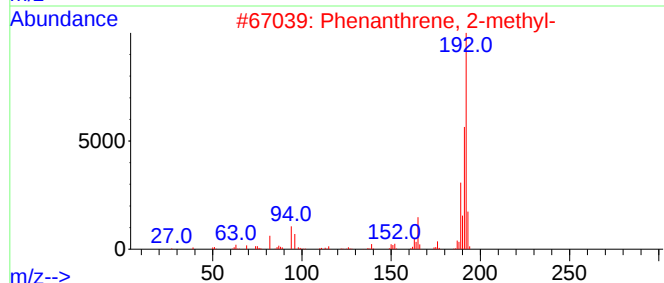
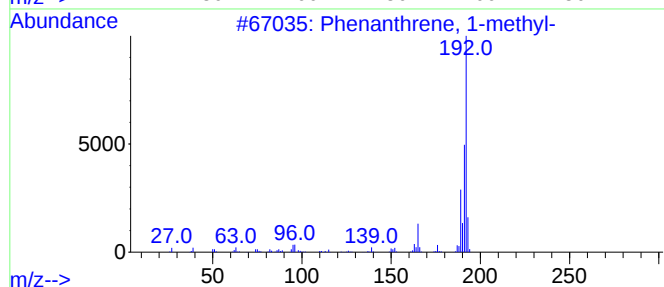
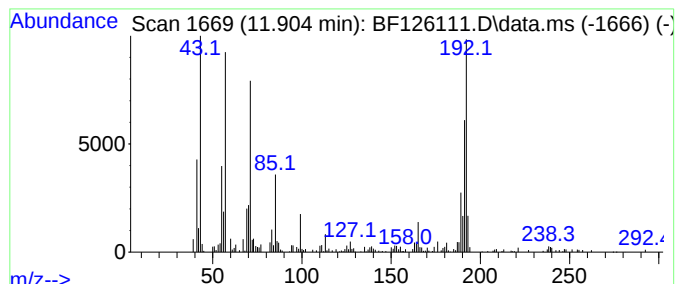
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Phenanthrene, 1-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.92 ng	284836	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
Acq On : 10 Nov 2021 17:09
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Instrument :
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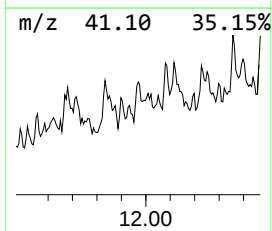
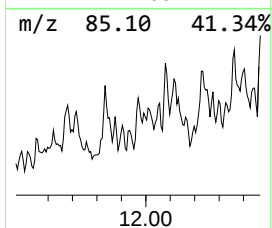
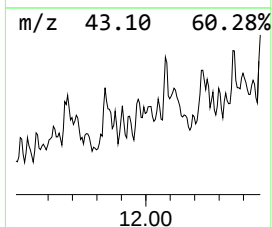
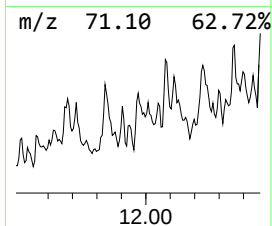
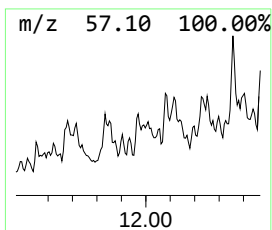
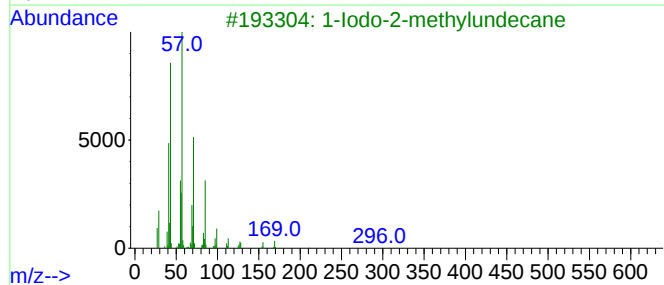
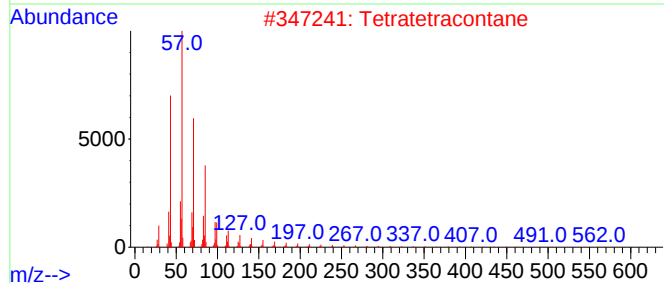
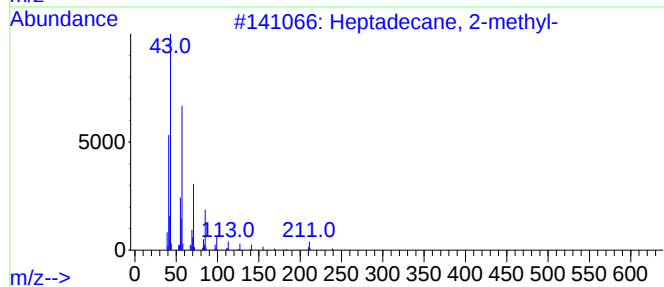
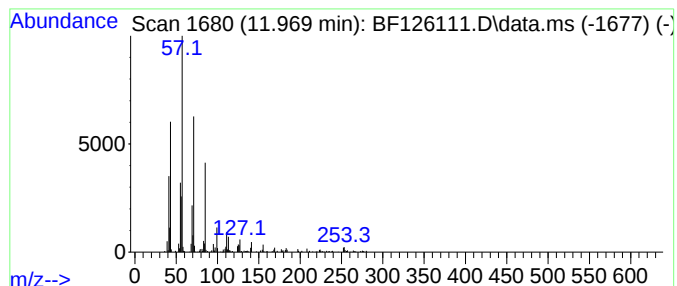
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heptadecane, 2-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	5.34 ng	309292	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
2			Tetratetracontane	619	C44H90	007098-22-8	72
3			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	72
4			Tridecane, 2-methyl-	198	C14H30	001560-96-9	72
5			Octacosane	394	C28H58	000630-02-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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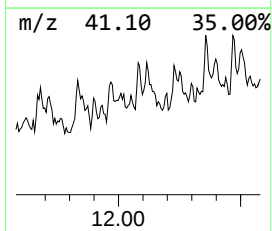
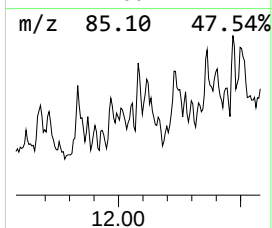
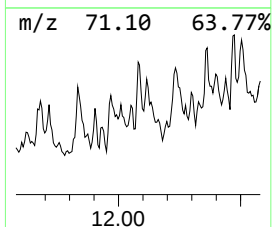
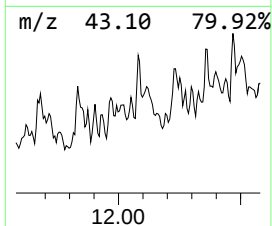
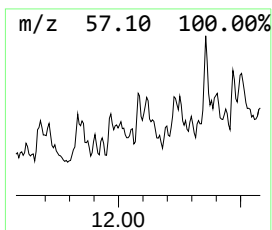
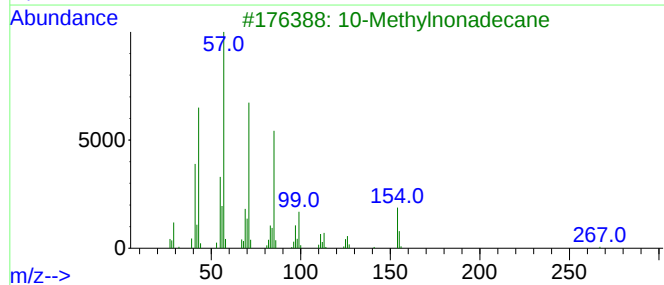
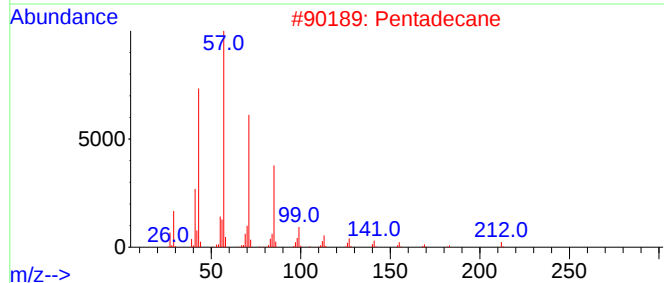
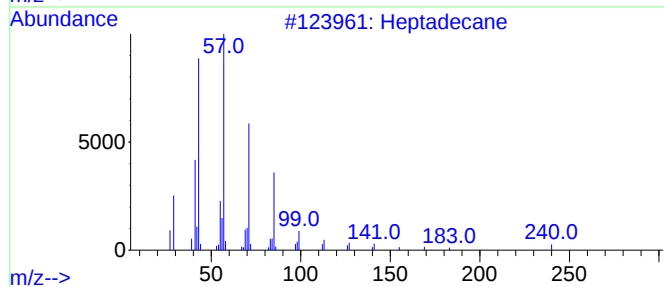
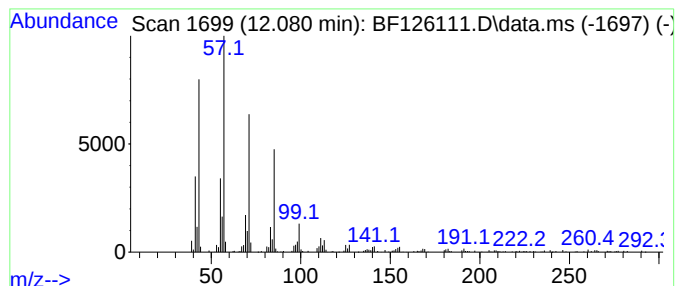
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.080	8.04 ng	465614	Phenanthrene-d10	11.374

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	87
2		Pentadecane	212	C15H32	000629-62-9	87
3		10-Methylnonadecane	282	C20H42	056862-62-5	86
4		Tetradecane	198	C14H30	000629-59-4	86
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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Acq On : 10 Nov 2021 17:09
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Sample : M4595-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

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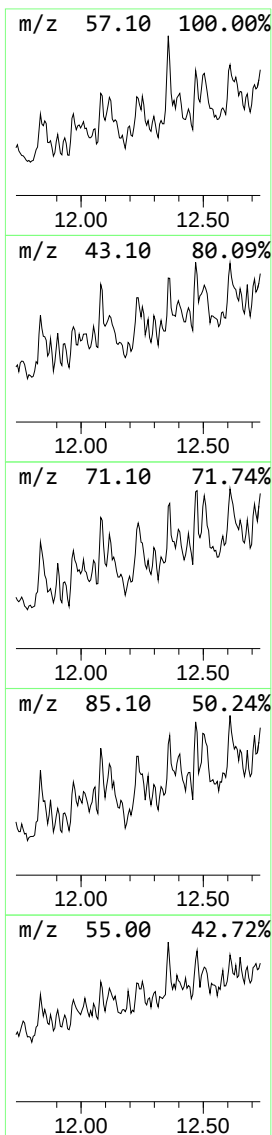
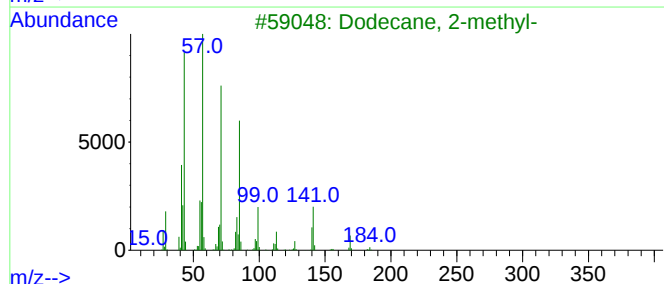
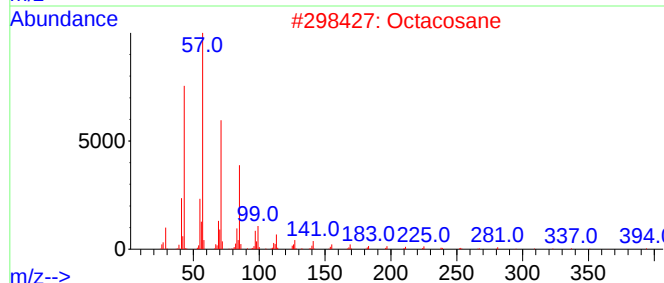
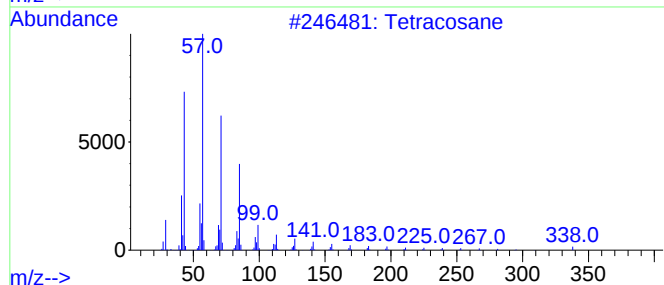
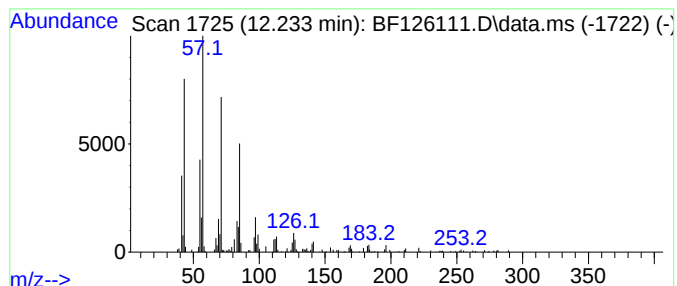
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	6.04 ng	349603	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	80
2			Octacosane	394	C28H58	000630-02-4	80
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
5			Undecane, 2-methyl-	170	C12H26	007045-71-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
Acq On : 10 Nov 2021 17:09
Operator : JU/CG
Sample : M4595-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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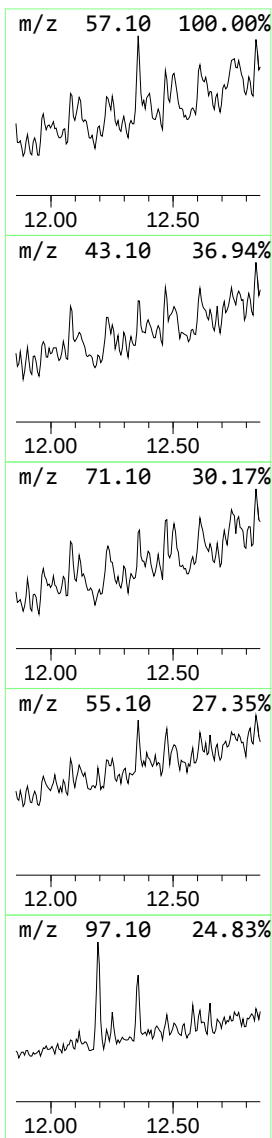
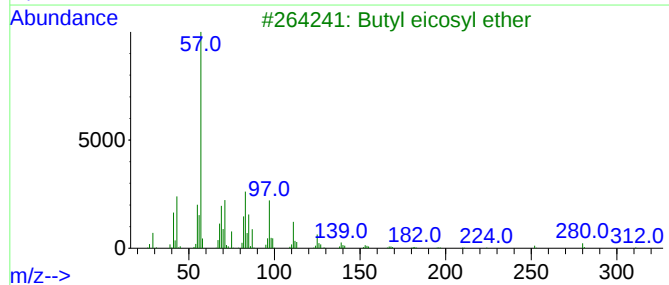
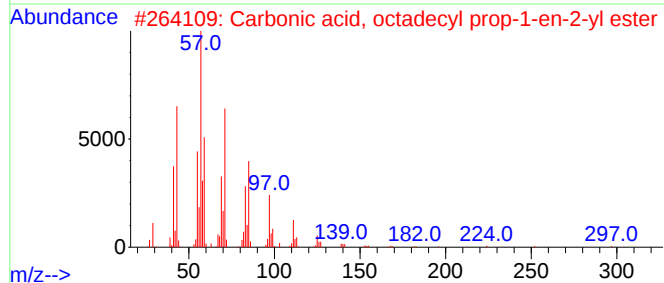
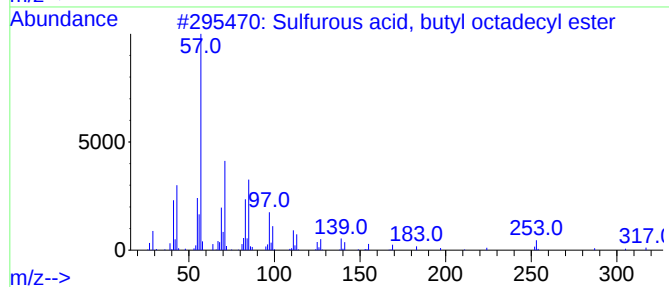
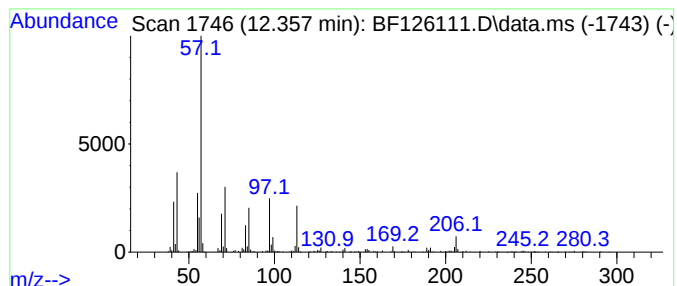
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Sulfurous acid, butyl octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	13.33 ng	772034	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	50
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	50
3			Butyl eicosyl ether	354	C24H50O	1000406-40-7	50
4			Tetratetracontane	619	C44H90	007098-22-8	43
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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Sample : M4595-08
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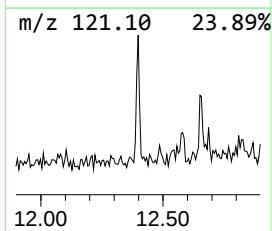
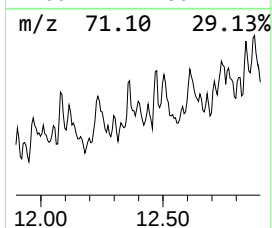
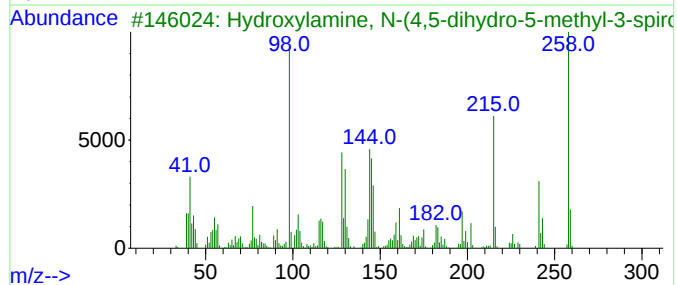
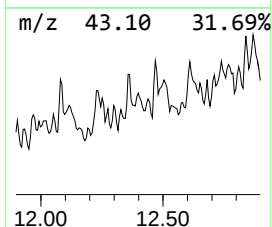
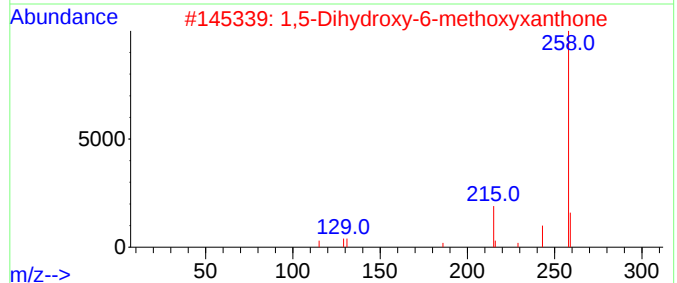
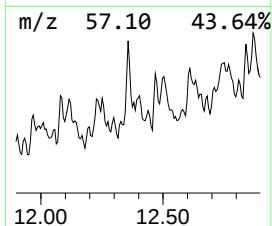
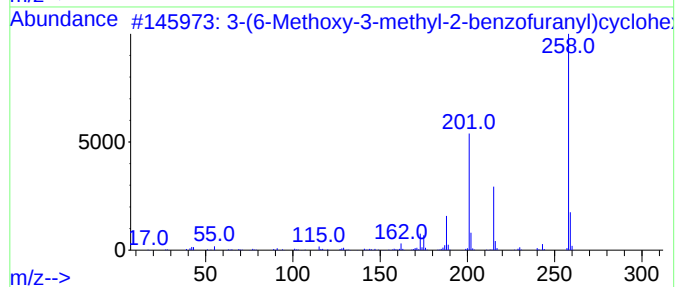
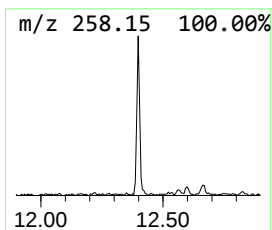
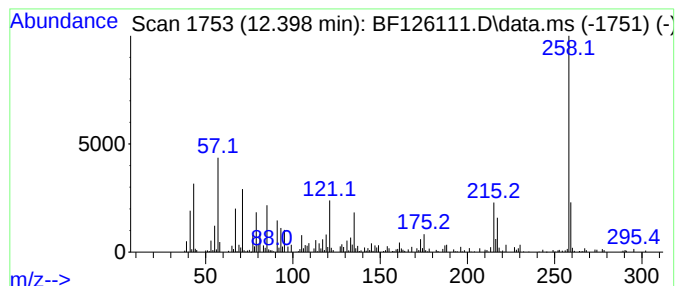
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 3-(6-Methoxy-3-methyl-2-ben... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.398	5.62 ng	325364	Phenanthrene-d10			11.374
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-(6-Methoxy-3-methyl-2-benzofur...		258	C16H18O3	1000239-79-6	64
2	1,5-Dihydroxy-6-methoxyxanthone		258	C14H10O5	181307-35-7	59
3	Hydroxylamine, N-(4,5-dihydro-5-...		258	C16H22N2O	1000274-03-9	58
4	Buchanaxanthone		258	C14H10O5	020081-65-6	50
5	Dibenzo[b,h][1,6]naphthyridine, ...		258	C18H14N2	004240-85-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
Acq On : 10 Nov 2021 17:09
Operator : JU/CG
Sample : M4595-08
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Instrument :
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ClientSampleId :
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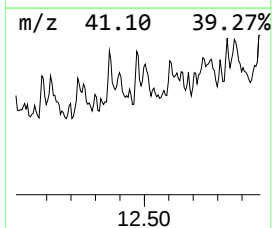
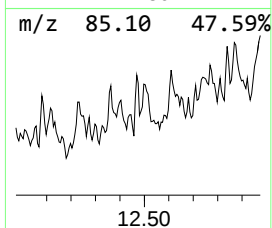
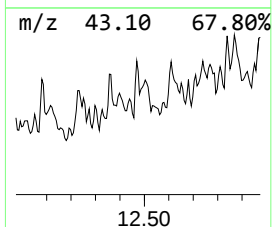
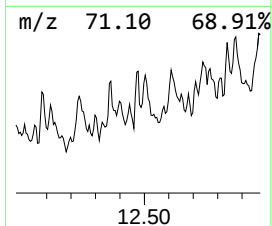
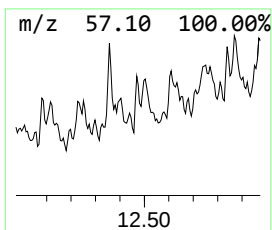
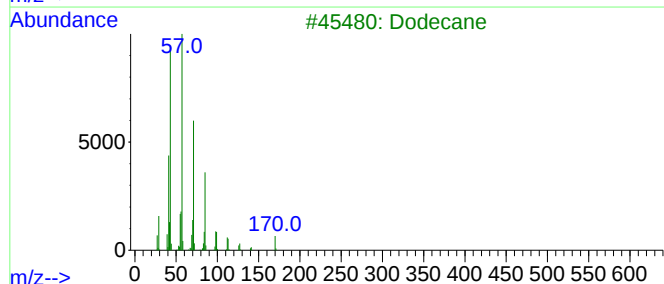
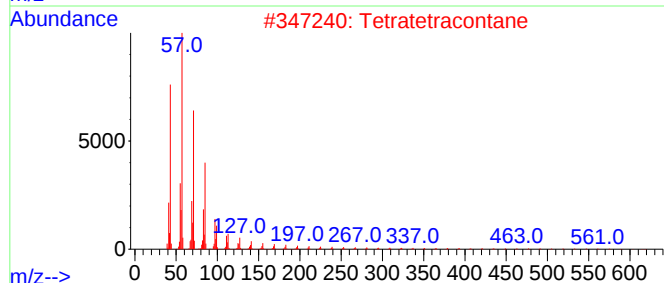
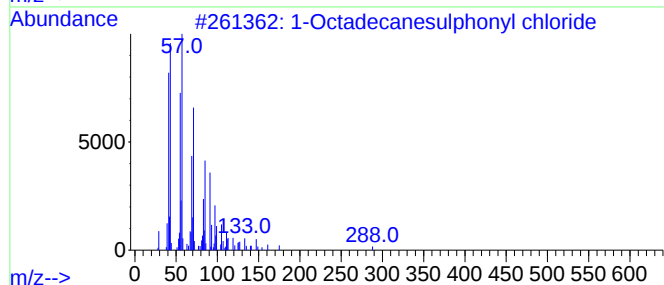
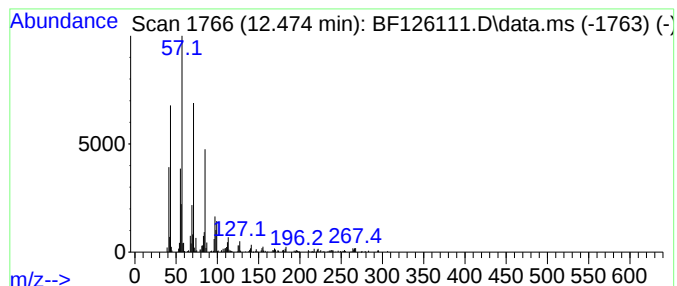
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	9.01 ng	522123	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
2			Tetratetracontane	619	C44H90	007098-22-8	86
3			Dodecane	170	C12H26	000112-40-3	83
4			Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5			Tetradecane	198	C14H30	000629-59-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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Acq On : 10 Nov 2021 17:09
Operator : JU/CG
Sample : M4595-08
Misc :
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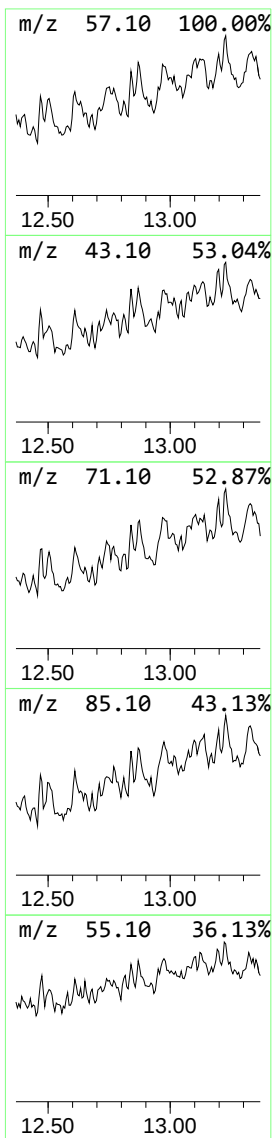
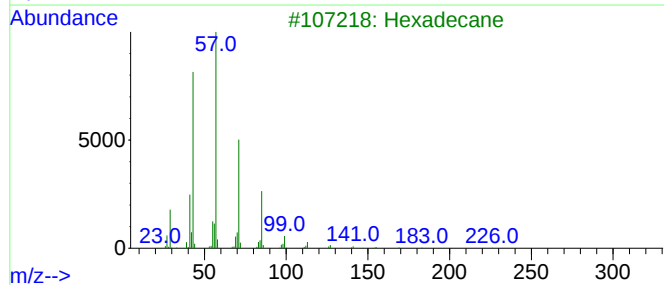
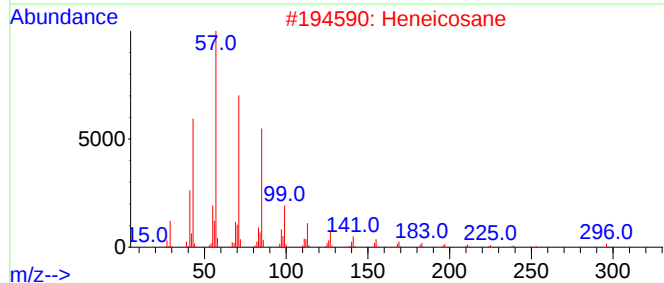
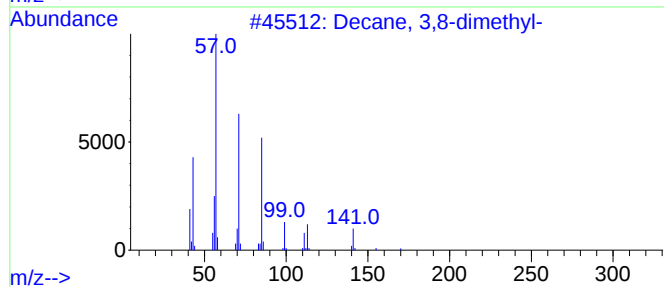
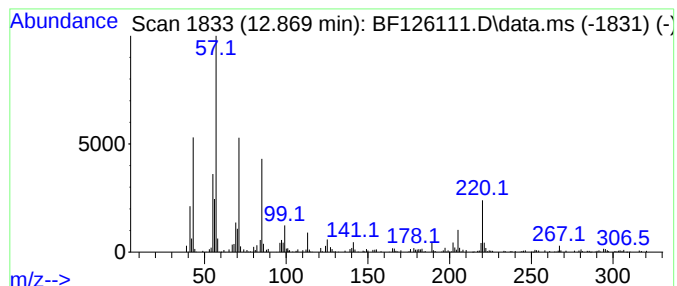
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Decane, 3,8-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.868	8.51 ng	581478	Chrysene-d12		14.015	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	90
2	Heneicosane		296	C21H44	000629-94-7	83
3	Hexadecane		226	C16H34	000544-76-3	70
4	Nonadecane		268	C19H40	000629-92-5	64
5	Decane, 1-iodo-		268	C10H21I	002050-77-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
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Sample : M4595-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CMC-ICS-003-004

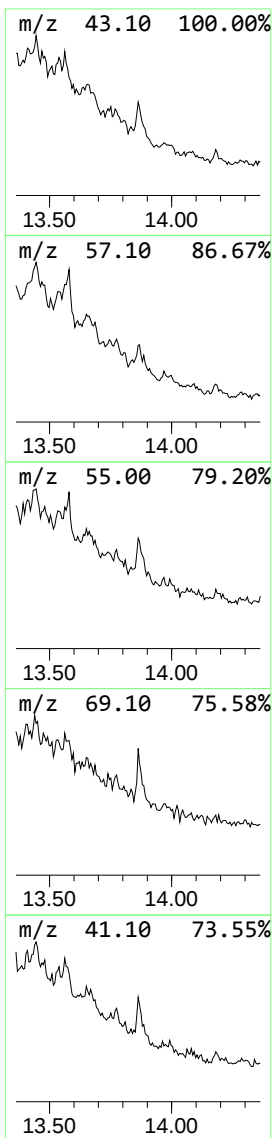
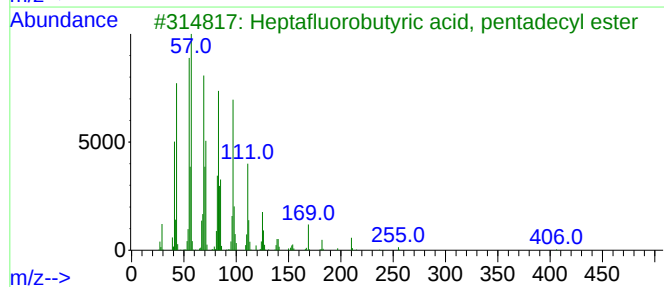
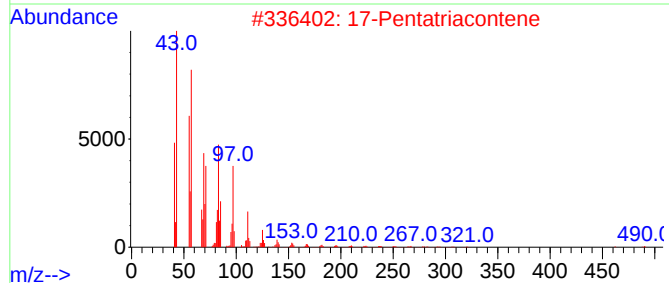
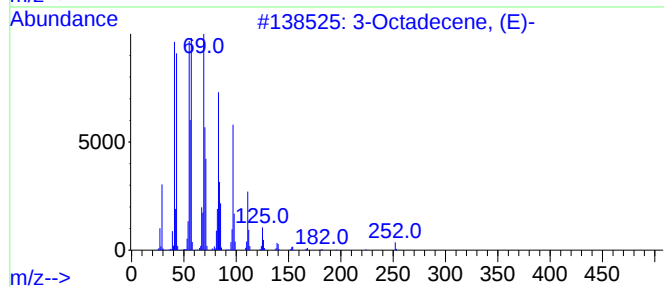
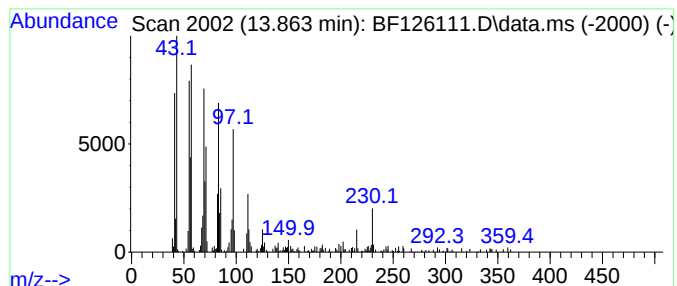
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	12.57 ng	858854	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octadecene, (E)-	252	C18H36	007206-19-1	93
2			17-Pentatriacontene	491	C35H70	006971-40-0	90
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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Data File : BF126111.D
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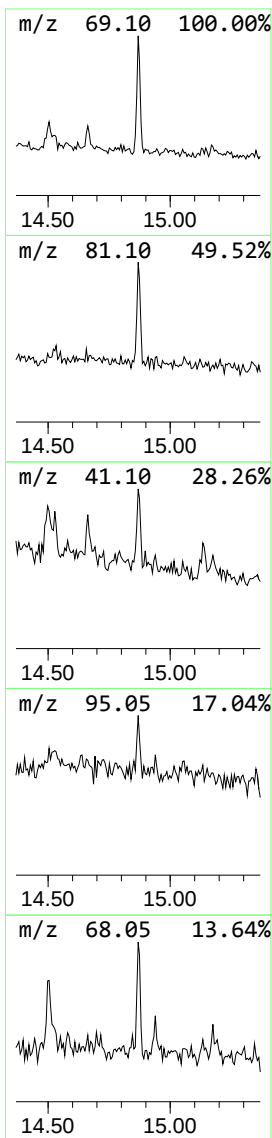
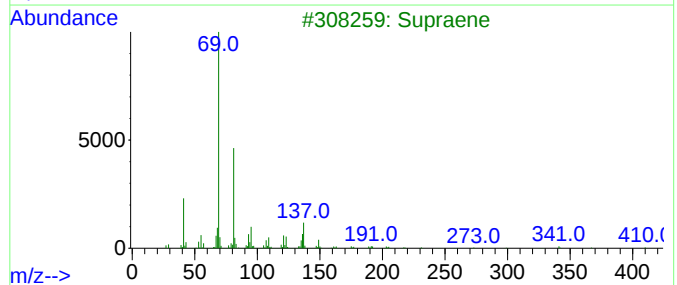
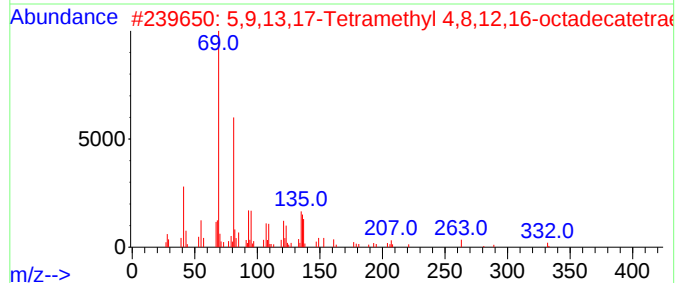
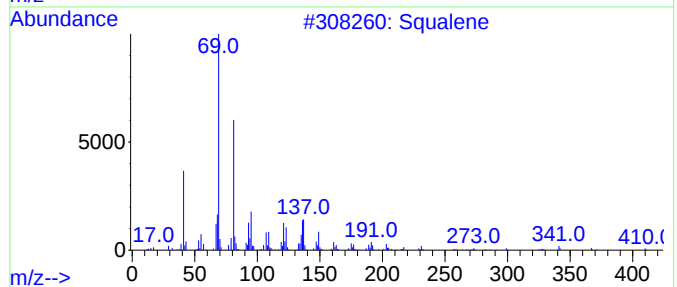
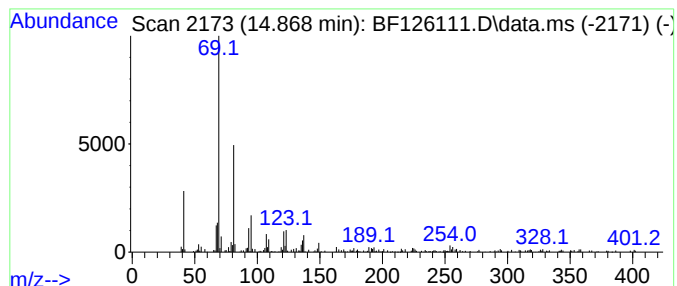
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Squalene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	5.47 ng	200366	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	64
2			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	64
3			Supraene	410	C30H50	007683-64-9	59
4			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	59
5			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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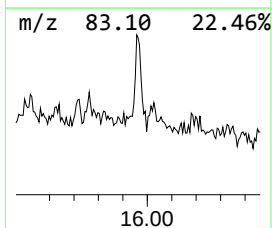
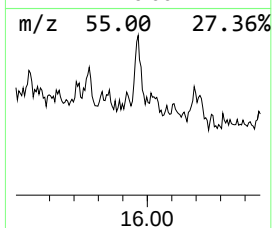
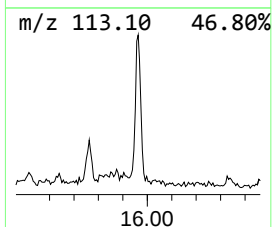
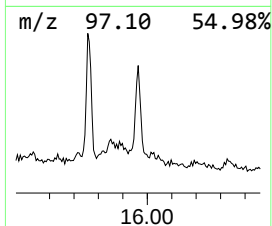
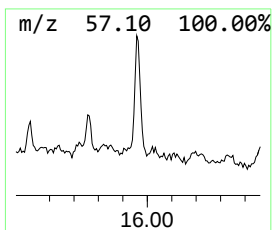
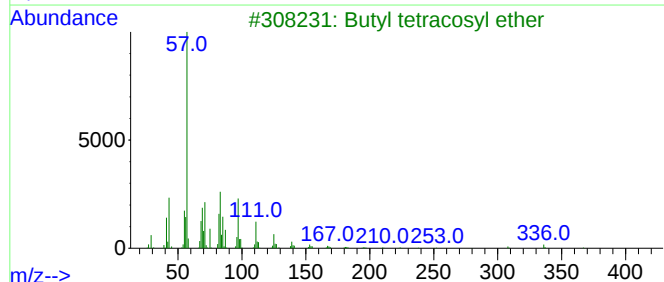
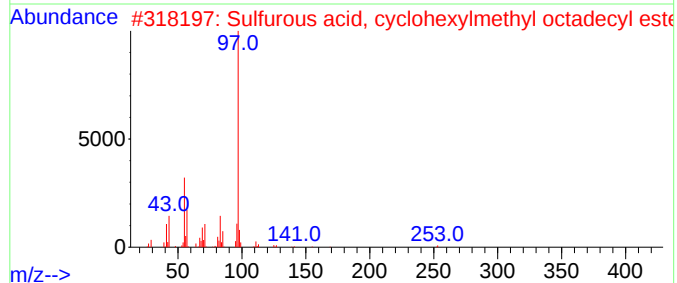
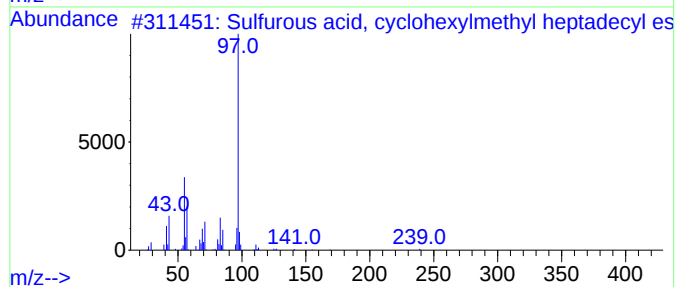
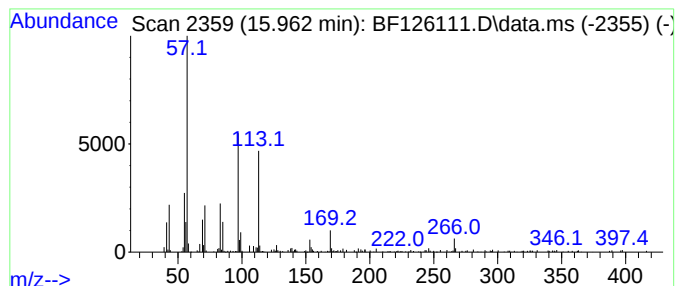
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown15.962 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.962	11.19 ng	409872	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	38
2			Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	38
3			Butyl tetracosyl ether	410	C28H58O	1000406-40-9	32
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	27
5			Fumaric acid, 2-decyl pentadecyl...	466	C29H54O4	1000348-59-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126111.D
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CMC-ICS-003-004

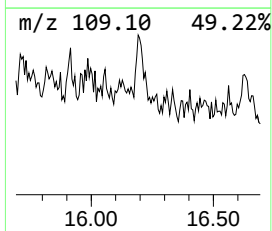
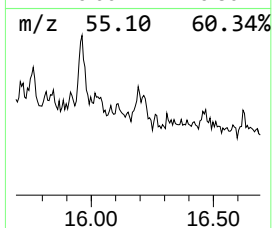
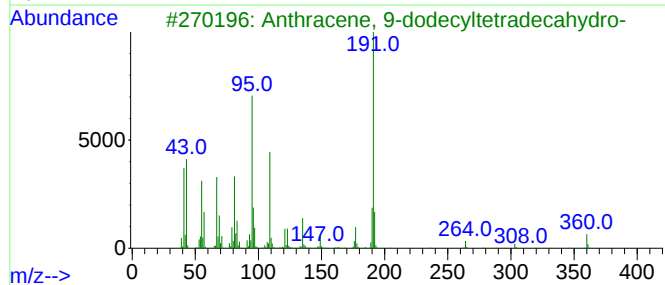
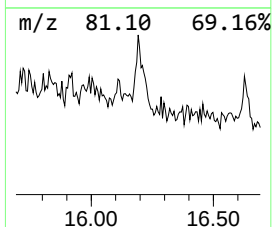
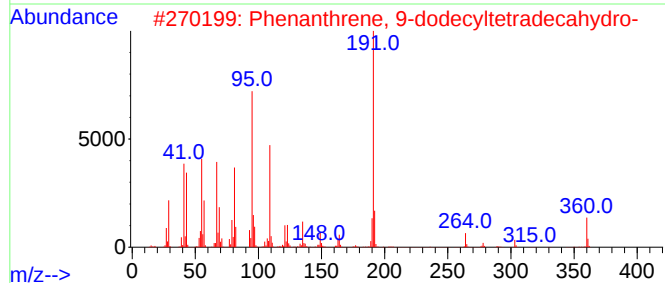
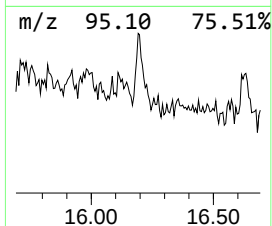
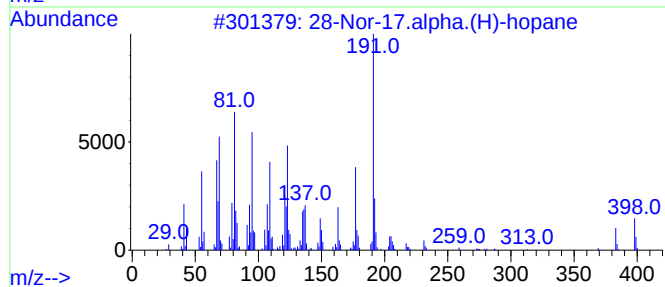
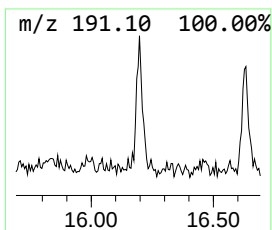
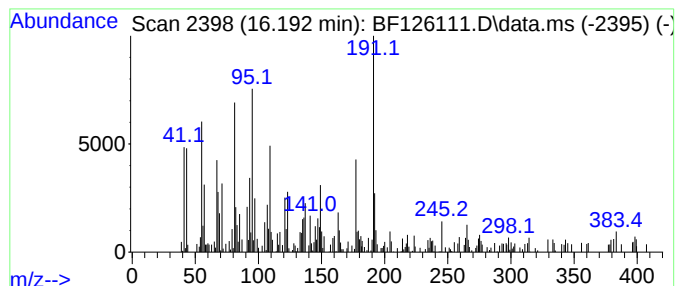
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 28-Nor-17.alpha.(H)-hopane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	5.64 ng	206473	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	72
2			Phenanthrene, 9-dodecyltetradeca...	360	C26H48	055334-01-5	70
3			Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	68
4			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	50
5			2,3,3,4,4,6,6,7,7,8-Decamethyl-5...	334	C14H38OSi4	1000424-58-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
 Data File : BF126111.D
 Acq On : 10 Nov 2021 17:09
 Operator : JU/CG
 Sample : M4595-08
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CMC-ICS-003-004

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	41.5	ng	2193000	1	6.851	1057330	20.0
3-Penten-2-one,...	4.451	22.1	ng	1168570	1	6.851	1057330	20.0
2-Pentanone, 4-...	5.081	58.8	ng	3110570	1	6.851	1057330	20.0
Ethanol, 2-(2-b...	8.039	11.3	ng	709018	2	8.134	1251140	20.0
Sulfurous acid,...	11.275	6.6	ng	380123	4	11.374	1158560	20.0
Octadecane, 2-m...	11.557	5.7	ng	330061	4	11.374	1158560	20.0
Undecane, 2-met...	11.680	11.1	ng	642432	4	11.374	1158560	20.0
Sulfurous acid,...	11.833	6.0	ng	348999	4	11.374	1158560	20.0
Phenanthrene, 1...	11.904	4.9	ng	284836	4	11.374	1158560	20.0
Heptadecane, 2-...	11.969	5.3	ng	309292	4	11.374	1158560	20.0
Heptadecane	12.080	8.0	ng	465614	4	11.374	1158560	20.0
Tetracosane	12.233	6.0	ng	349603	4	11.374	1158560	20.0
Sulfurous acid,...	12.357	13.3	ng	772034	4	11.374	1158560	20.0
3-(6-Methoxy-3-...	12.398	5.6	ng	325364	4	11.374	1158560	20.0
1-Octadecanesul...	12.474	9.0	ng	522123	4	11.374	1158560	20.0
Decane, 3,8-dim...	12.868	8.5	ng	581478	5	14.015	1365970	20.0
3-Octadecene, (E)-	13.863	12.6	ng	858854	5	14.015	1365970	20.0
Squalene	14.868	5.5	ng	200366	6	15.480	732580	20.0
unknown15.962	15.962	11.2	ng	409872	6	15.480	732580	20.0
28-Nor-17.alpha...	16.192	5.6	ng	206473	6	15.480	732580	20.0