

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
 Data File : BF126353.D
 Acq On : 23 Dec 2021 19:49
 Operator : JU/CG
 Sample : M5191-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-(3.5-7.0)-12-21-2021

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.869	295	303	309	rBV2	14110	22179	1.07%	0.107%
2	4.393	389	392	397	rBV	26083	30868	1.49%	0.149%
3	5.016	492	498	508	rBV	218109	278217	13.44%	1.345%
4	5.428	563	568	579	rBV	2091037	2034121	98.25%	9.832%
5	6.439	736	740	752	rBV	1957894	2070250	100.00%	10.007%
6	6.816	800	804	807	rBV	791571	613369	29.63%	2.965%
7	7.375	890	899	902	rBV	1553365	1314030	63.47%	6.351%
8	7.416	904	906	910	rVB	31687	28627	1.38%	0.138%
9	8.098	1017	1022	1025	rBV	850781	735336	35.52%	3.554%
10	8.528	1091	1095	1100	rBV	44233	41803	2.02%	0.202%
11	8.698	1120	1124	1128	rVB	68619	58648	2.83%	0.283%
12	9.128	1194	1197	1201	rVB	53500	42815	2.07%	0.207%
13	9.175	1201	1205	1208	rBV	2234650	1821799	88.00%	8.806%
14	9.257	1216	1219	1224	rBV	104362	109593	5.29%	0.530%
15	9.322	1228	1230	1236	rVB6	14852	21771	1.05%	0.105%
16	9.516	1259	1263	1265	rBV2	23844	22282	1.08%	0.108%
17	9.580	1269	1274	1276	rBV2	62349	72443	3.50%	0.350%
18	9.727	1294	1299	1302	rBV4	15224	31189	1.51%	0.151%
19	9.792	1307	1310	1314	rVV	83522	71441	3.45%	0.345%
20	9.851	1314	1320	1324	rVV	861572	700602	33.84%	3.386%
21	9.886	1324	1326	1329	rVB	36120	28636	1.38%	0.138%
22	10.027	1343	1350	1352	rBV4	11983	25458	1.23%	0.123%
23	10.057	1352	1355	1357	rVB2	25636	24533	1.19%	0.119%
24	10.263	1387	1390	1392	rBV2	24000	25234	1.22%	0.122%
25	10.286	1392	1394	1397	rVB	67516	58077	2.81%	0.281%
26	10.510	1429	1432	1435	rVV	42044	39316	1.90%	0.190%
27	10.563	1437	1441	1444	rVB4	18131	22836	1.10%	0.110%
28	10.639	1450	1454	1458	rBV	931641	820885	39.65%	3.968%
29	10.763	1472	1475	1476	rBV	76563	61366	2.96%	0.297%
30	11.204	1544	1550	1553	rBV2	146841	172124	8.31%	0.832%
31	11.239	1553	1556	1558	rVV2	52757	61366	2.96%	0.297%
32	11.263	1558	1560	1563	rVB	36472	29451	1.42%	0.142%
33	11.339	1569	1573	1575	rBV	818911	717248	34.65%	3.467%
34	11.363	1575	1577	1580	rVV	288441	231889	11.20%	1.121%
35	11.410	1580	1585	1589	rVB2	76682	96307	4.65%	0.466%
36	11.504	1600	1601	1607	rVB3	19159	24147	1.17%	0.117%

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37	11.569	1607	1612	1614	rBV2	33236	40162	1.94%	0.194%
38	11.639	1621	1624	1627	rBV	55450	45776	2.21%	0.221%
39	11.739	1638	1641	1648	rVB7	30067	42140	2.04%	0.204%
40	11.804	1648	1652	1655	rBV4	19464	34180	1.65%	0.165%
41	11.839	1655	1658	1660	rBV	40266	35812	1.73%	0.173%
42	11.869	1660	1663	1667	rVB	84298	65347	3.16%	0.316%
43	11.904	1667	1669	1672	rBV2	37553	38981	1.88%	0.188%
44	11.951	1672	1677	1679	rBV2	68561	95604	4.62%	0.462%
45	12.021	1686	1689	1691	rBV	45314	48753	2.35%	0.236%
46	12.045	1691	1693	1696	rVB	48122	38440	1.86%	0.186%
47	12.157	1710	1712	1717	rVB5	29697	34792	1.68%	0.168%
48	12.321	1737	1740	1743	rBV3	36447	51798	2.50%	0.250%
49	12.386	1747	1751	1754	rBV3	47379	69570	3.36%	0.336%
50	12.433	1754	1759	1763	rVB3	71513	95721	4.62%	0.463%
51	12.474	1763	1766	1771	rBV2	38512	49206	2.38%	0.238%
52	12.551	1775	1779	1782	rBV	784948	664939	32.12%	3.214%
53	12.580	1782	1784	1793	rVB4	106259	185138	8.94%	0.895%
54	12.780	1811	1818	1821	rBV	703742	711274	34.36%	3.438%
55	12.827	1824	1826	1831	rVB3	52074	66092	3.19%	0.319%
56	12.898	1836	1838	1839	rBV	28271	21622	1.04%	0.105%
57	12.927	1839	1843	1846	rBV	2078791	1882534	90.93%	9.099%
58	12.992	1851	1854	1859	rBV3	58257	98402	4.75%	0.476%
59	13.110	1871	1874	1876	rVB	62557	57510	2.78%	0.278%
60	13.168	1881	1884	1887	rVB3	74406	85163	4.11%	0.412%
61	13.210	1888	1891	1894	rBV	62241	79421	3.84%	0.384%
62	13.410	1922	1925	1931	rVB	319227	287268	13.88%	1.389%
63	13.510	1939	1942	1944	rVB3	58681	48788	2.36%	0.236%
64	13.904	2005	2009	2017	rBV5	149967	418909	20.23%	2.025%
65	13.980	2017	2022	2024	rVV2	795379	1047331	50.59%	5.062%
66	14.004	2024	2026	2029	rVB	286343	224836	10.86%	1.087%
67	14.157	2049	2052	2056	rBV2	72285	84163	4.07%	0.407%
68	14.457	2101	2103	2106	rBV2	90678	80944	3.91%	0.391%
69	15.009	2194	2197	2207	rVB	236712	452004	21.83%	2.185%
70	15.309	2245	2248	2254	rVB	131467	166700	8.05%	0.806%
71	15.368	2255	2258	2264	rVB	171798	191066	9.23%	0.924%
72	15.433	2265	2269	2272	rBV	410289	487870	23.57%	2.358%

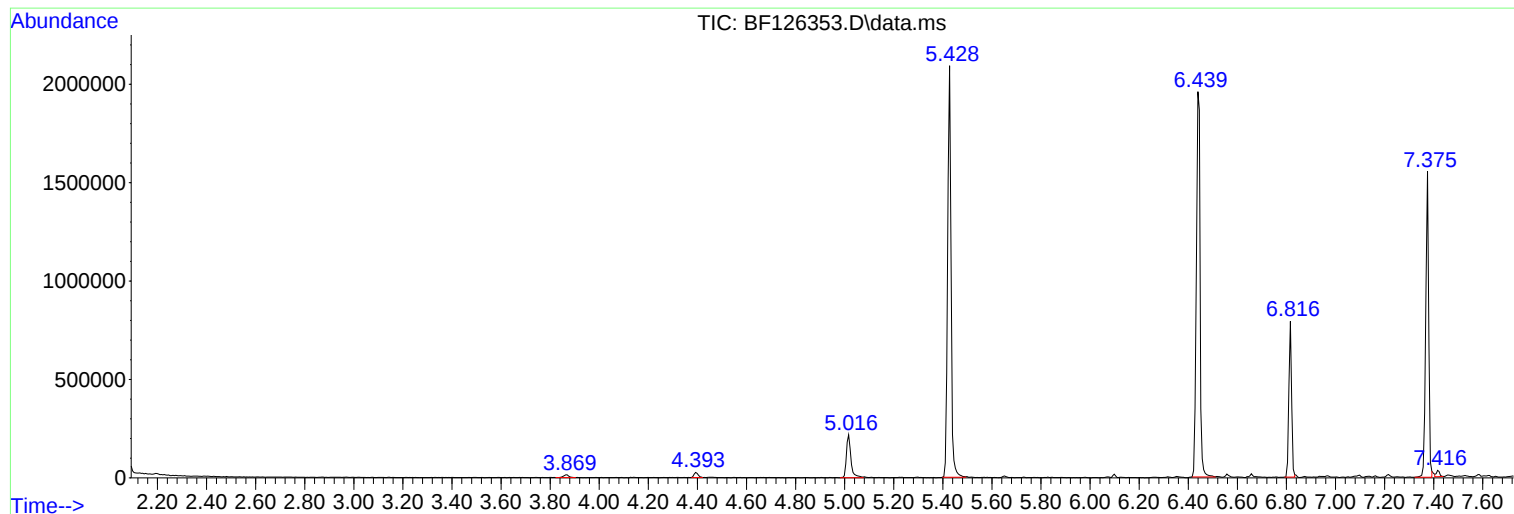
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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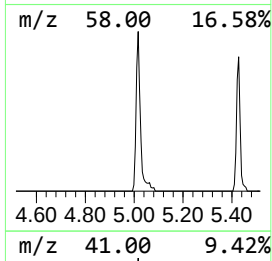
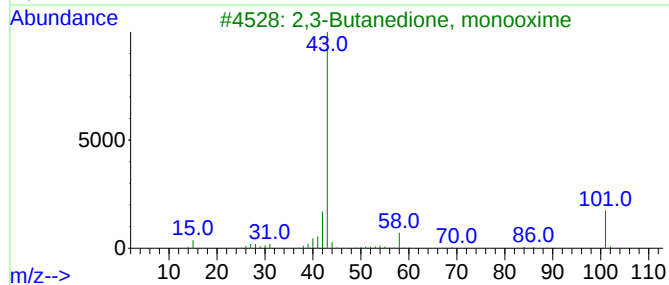
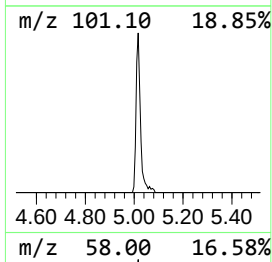
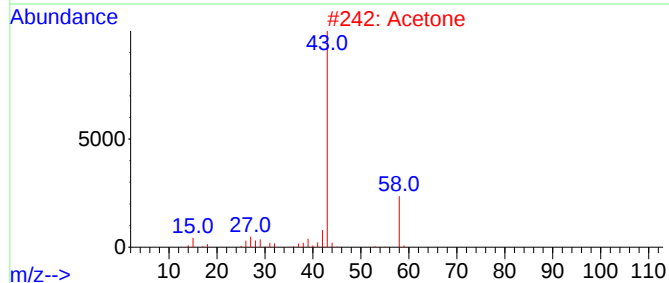
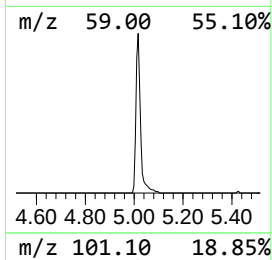
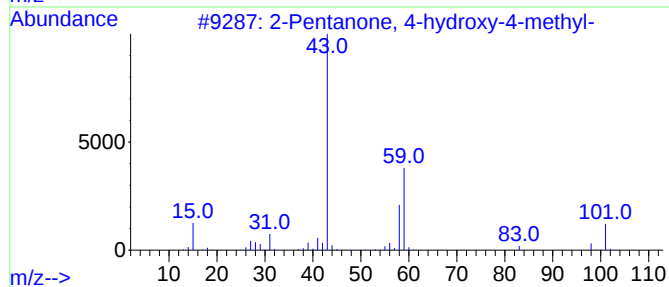
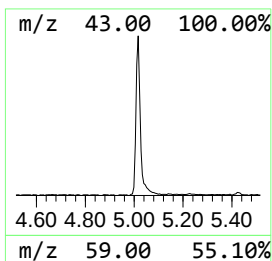
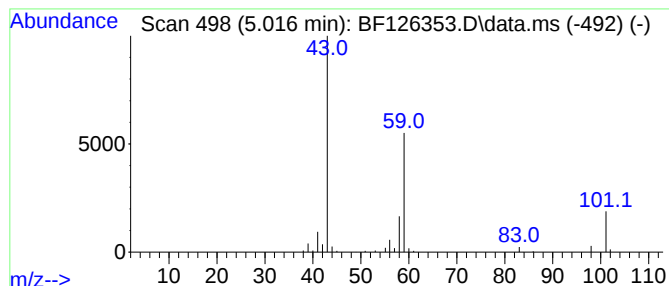
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.016	9.07 ng	278217	1,4-Dichlorobenzene-d4			6.816
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Acetone		58	C3H6O	000067-64-1	9
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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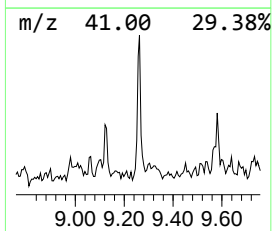
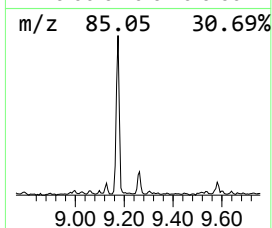
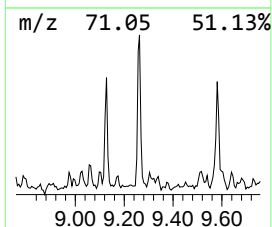
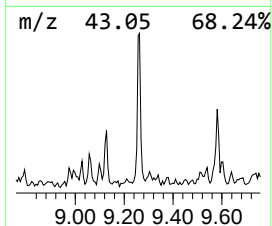
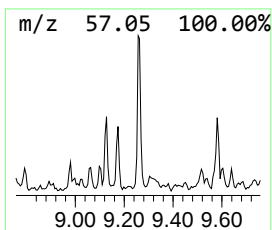
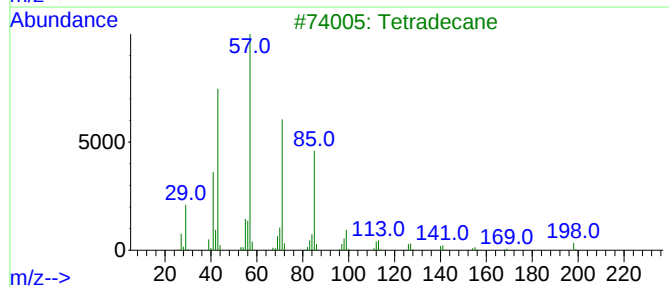
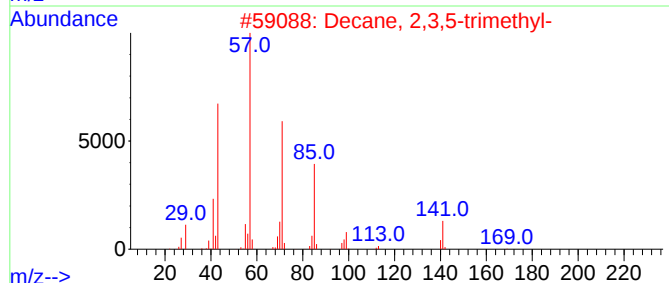
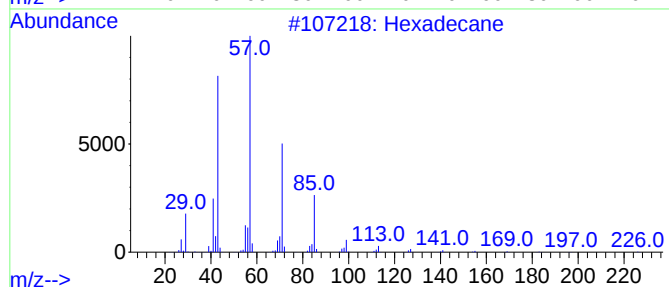
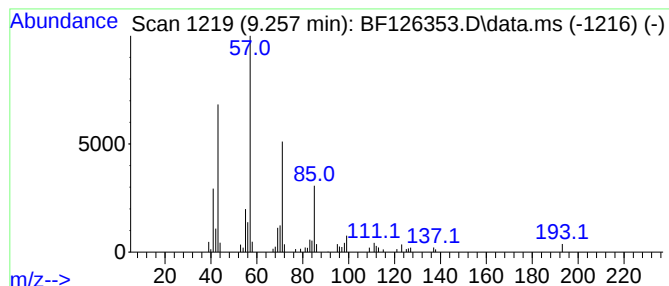
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	3.13 ng	109593	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	72
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
3			Tetradecane	198	C14H30	000629-59-4	64
4			Octacosane	394	C28H58	000630-02-4	59
5			Dodecane	170	C12H26	000112-40-3	59



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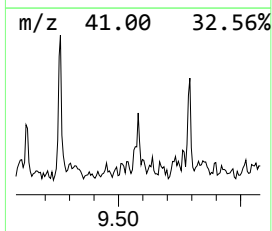
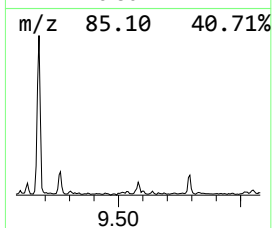
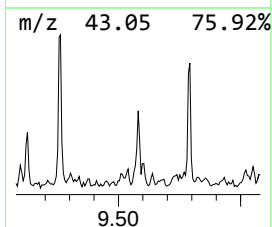
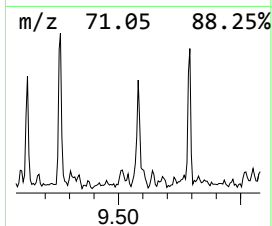
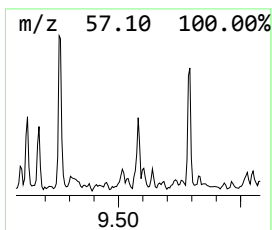
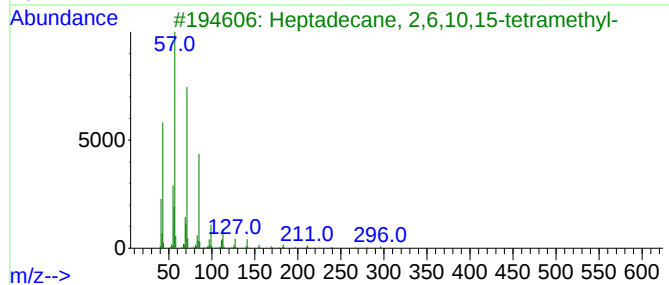
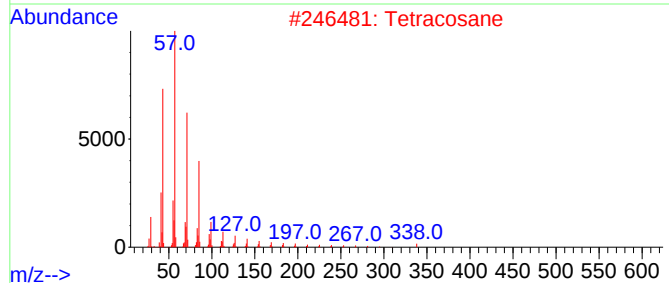
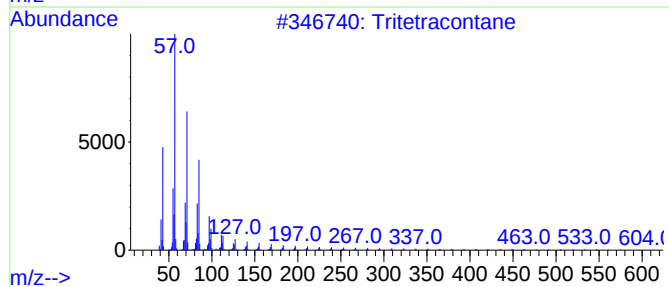
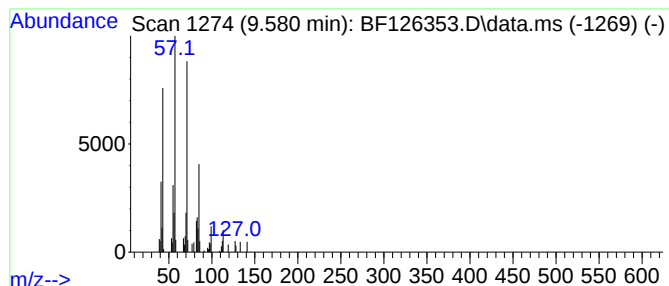
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Peak Number 3 Tritetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	2.07 ng	72443	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	83
2			Tetracosane	338	C24H50	000646-31-1	83
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
5			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72



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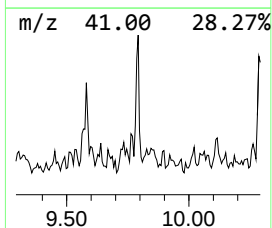
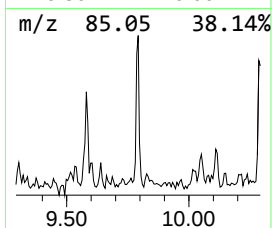
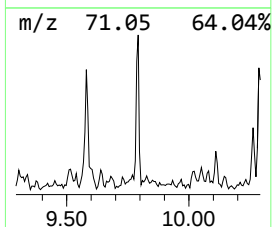
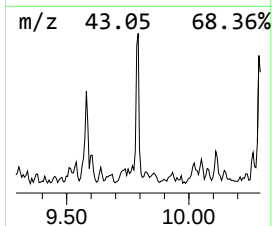
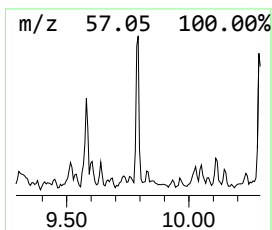
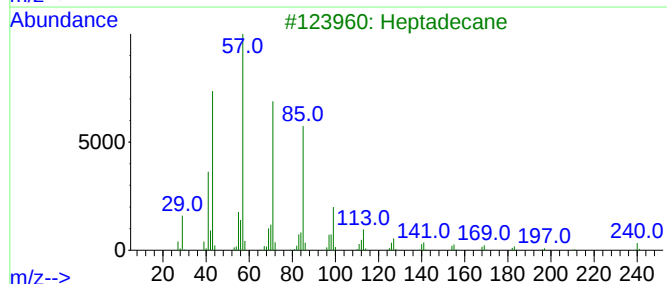
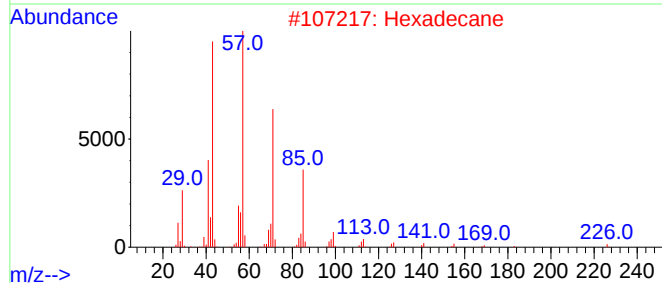
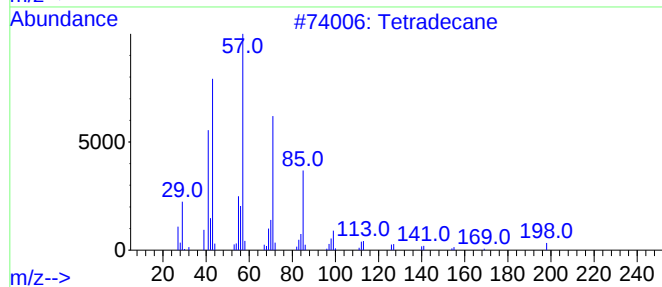
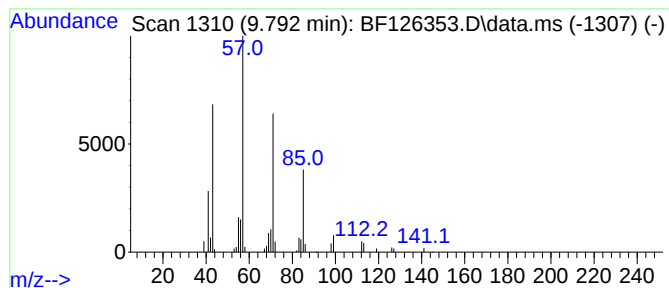
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.792	2.04 ng	71441	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Hexadecane	226	C16H34	000544-76-3	86
3			Heptadecane	240	C17H36	000629-78-7	83
4			Nonadecane	268	C19H40	000629-92-5	78
5			Tridecane	184	C13H28	000629-50-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
Data File : BF126353.D
Acq On : 23 Dec 2021 19:49
Operator : JU/CG
Sample : M5191-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-(3.5-7.0)-12-21-2021

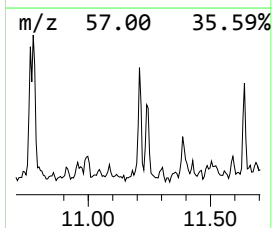
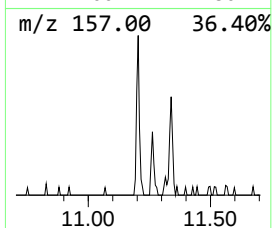
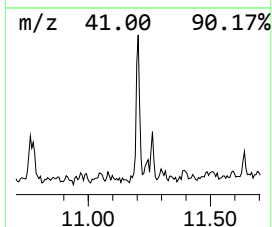
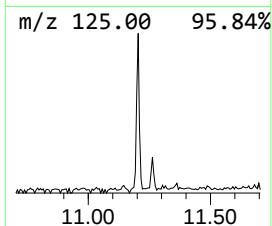
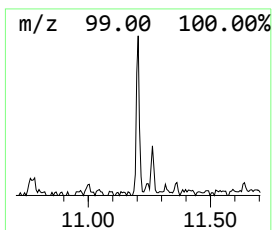
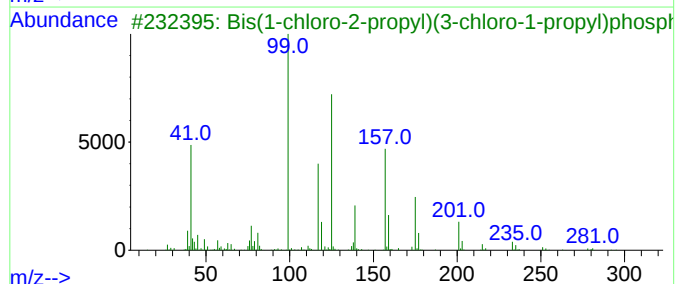
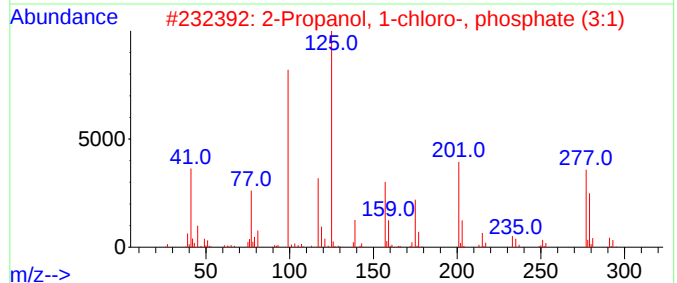
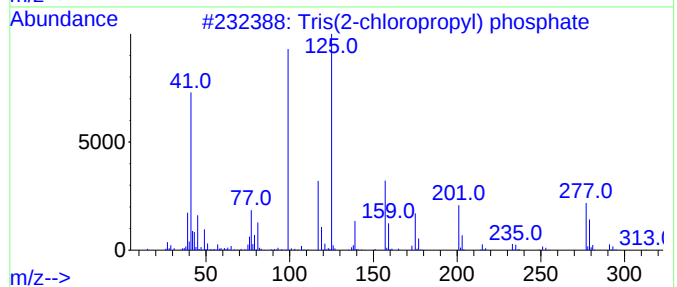
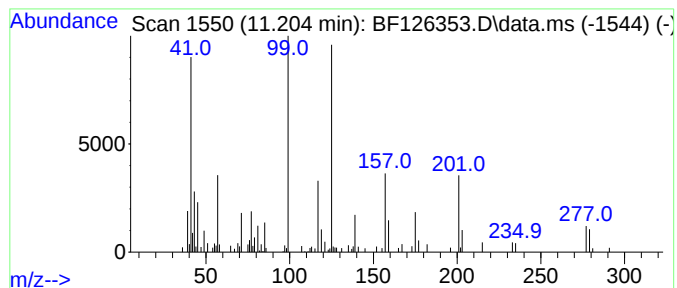
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tris(2-chloropropyl) phosphate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.204	4.80 ng	172124	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tris(2-chloropropyl) phosphate	326	C9H18Cl3O4P	006145-73-9	91
2			2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	90
3			Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	52
4			1,3-Dimethylbutyl methylphosphon...	182	C7H16F02P	000352-53-4	38
5			2-Butyl methylphosphonofluoridate	154	C5H12F02P	000352-52-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
Data File : BF126353.D
Acq On : 23 Dec 2021 19:49
Operator : JU/CG
Sample : M5191-03
Misc :
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Instrument :
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ClientSampleId :
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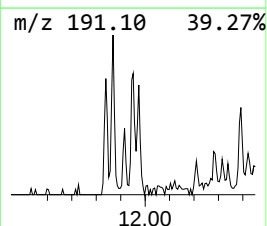
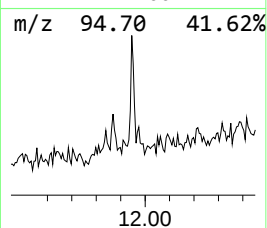
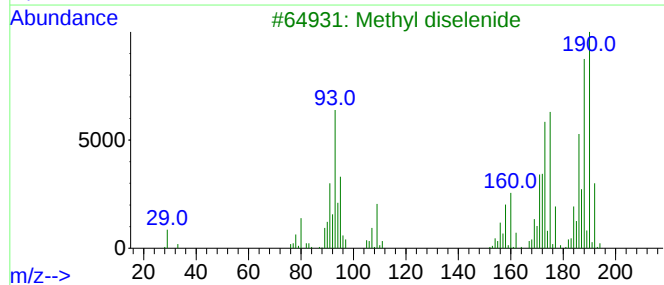
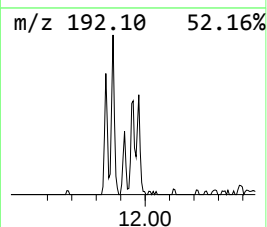
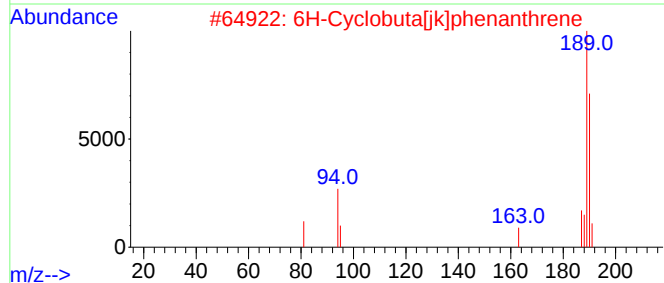
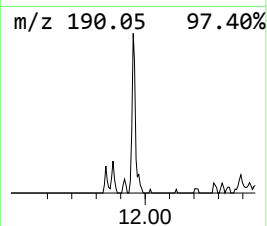
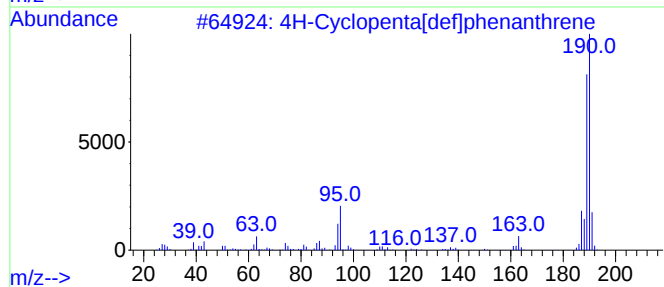
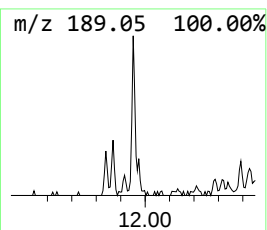
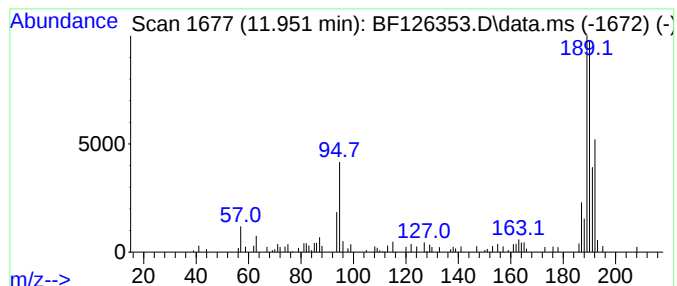
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.67 ng	95604	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3			Methyl diselenide	190	C2H6Se2	007101-31-7	38
4			Phenol, 4-(2-thienylmethyl)-	190	C11H10O5	091680-55-6	37
5			9,9'-Biphenanthrene, octacosahydro-	382	C28H46	055334-18-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
Data File : BF126353.D
Acq On : 23 Dec 2021 19:49
Operator : JU/CG
Sample : M5191-03
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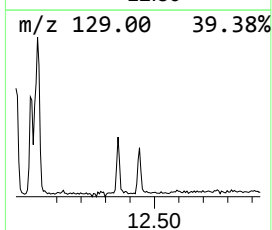
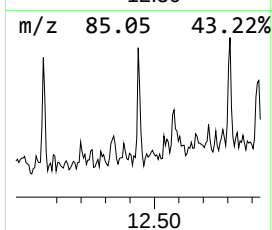
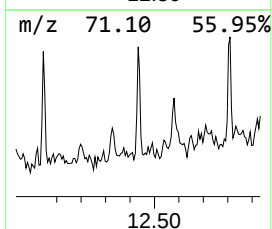
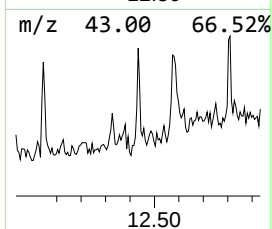
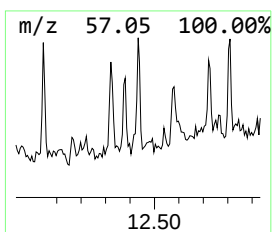
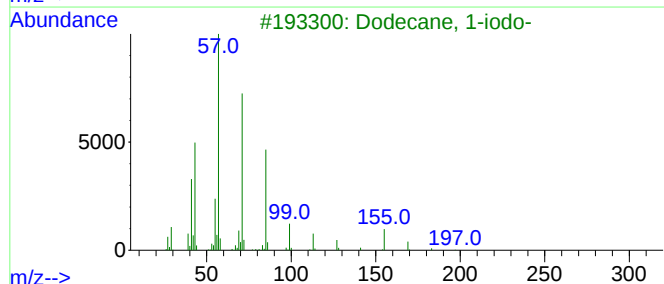
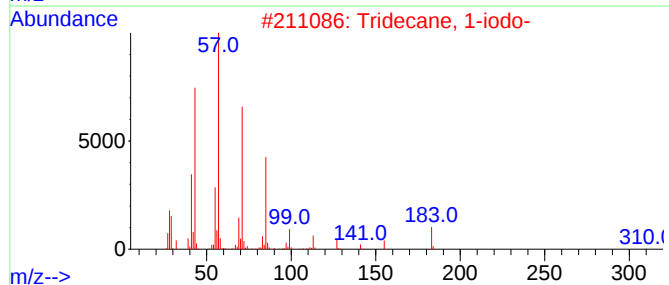
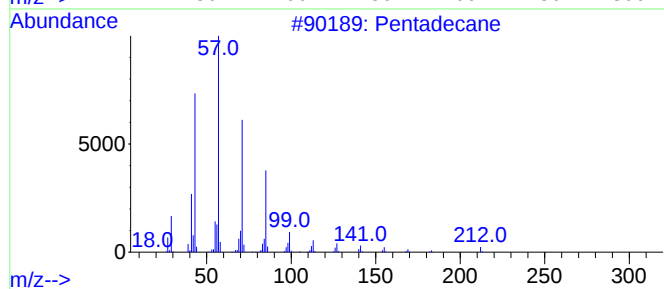
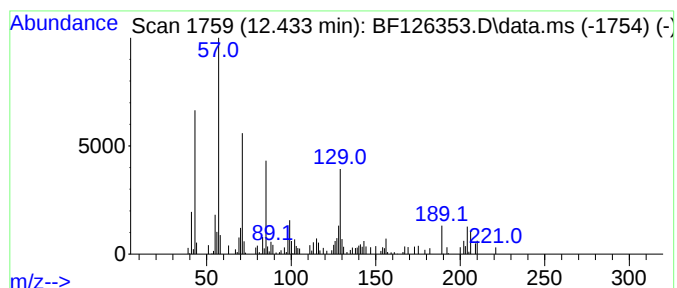
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ClientSampleId :
TP-(3.5-7.0)-12-21-2021

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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 unknown12.433 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.433	2.67 ng	95721	Phenanthrene-d10		11.339	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	43
2	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	38
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	38
4	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	38
5	Undecane, 3,9-dimethyl-		184	C13H28	017301-31-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
Data File : BF126353.D
Acq On : 23 Dec 2021 19:49
Operator : JU/CG
Sample : M5191-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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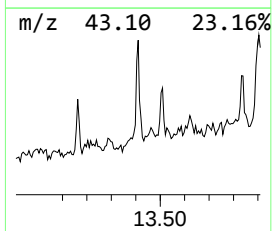
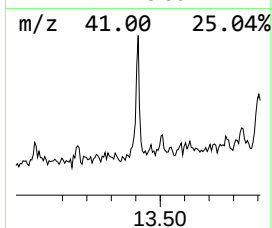
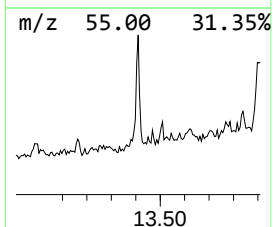
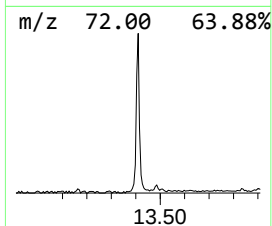
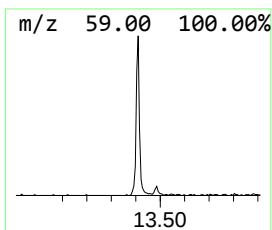
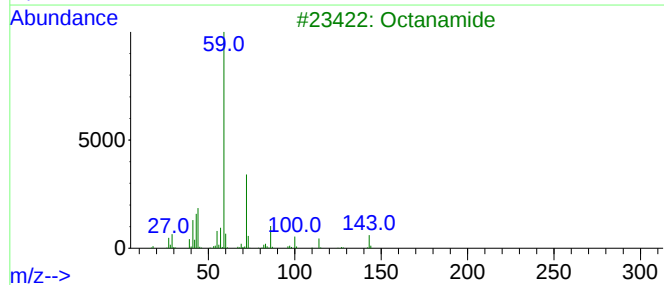
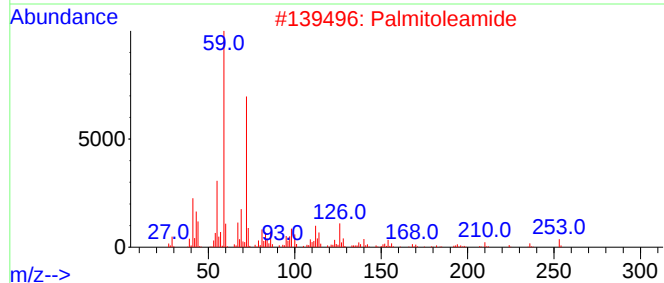
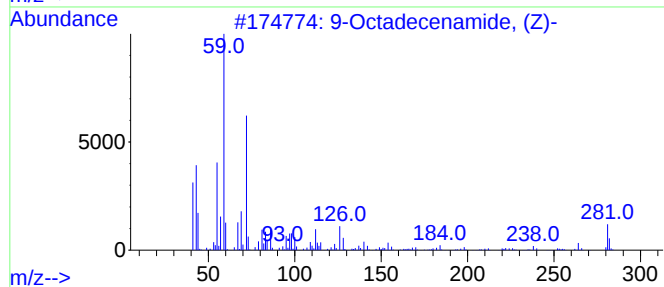
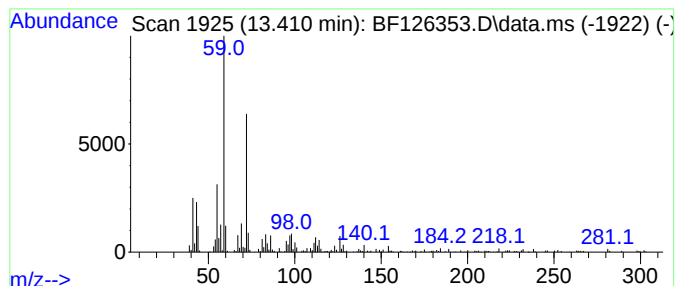
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	5.49 ng	287268	Chrysene-d12	13.980

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Palmitoleamide	253	C16H31NO	106010-22-4	83
3		Octanamide	143	C8H17NO	000629-01-6	72
4		7-Nonenamide	155	C9H17NO	090949-53-4	64
5		Hexadecanamide	255	C16H33NO	000629-54-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
Data File : BF126353.D
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Sample : M5191-03
Misc :
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Instrument :
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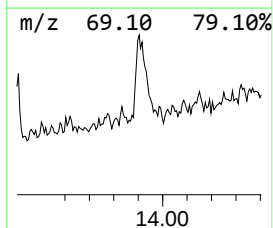
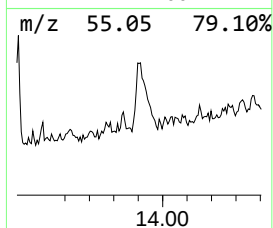
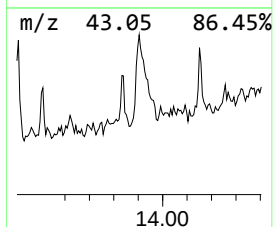
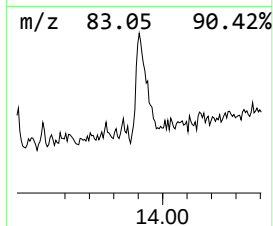
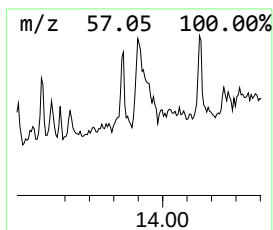
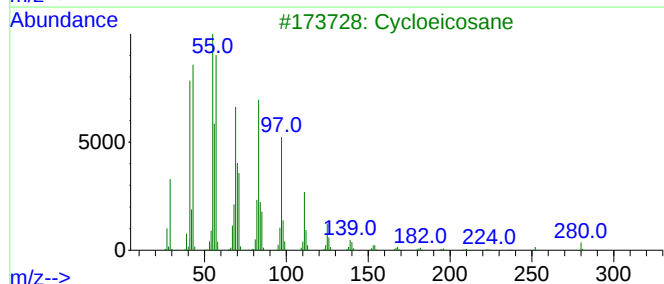
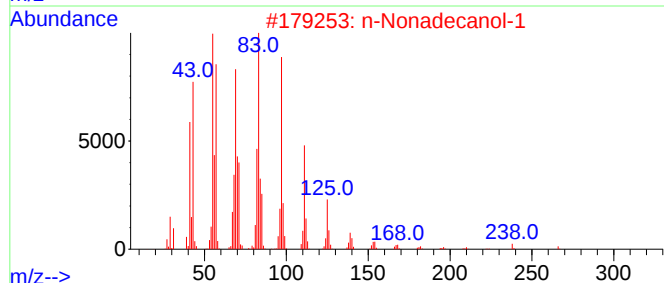
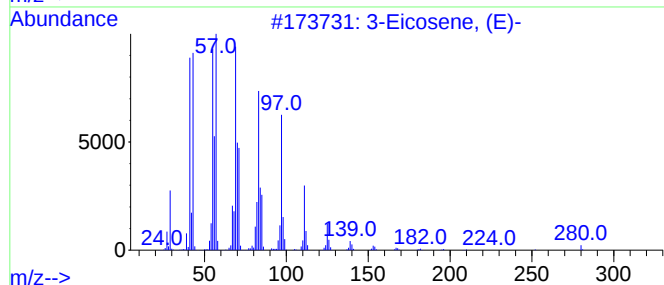
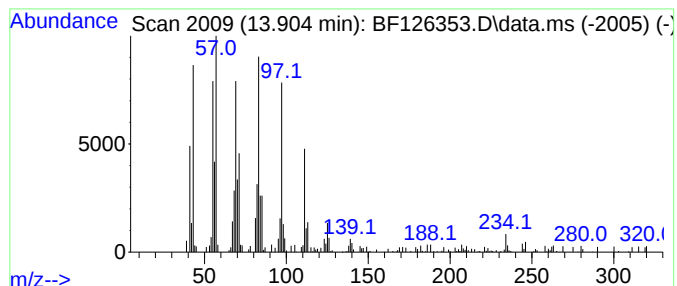
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	8.00 ng	418909	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			Cycloeicosane	280	C20H40	000296-56-0	83
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	83
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
Data File : BF126353.D
Acq On : 23 Dec 2021 19:49
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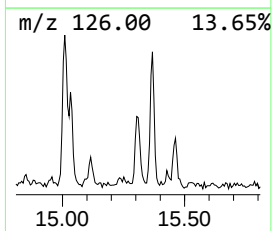
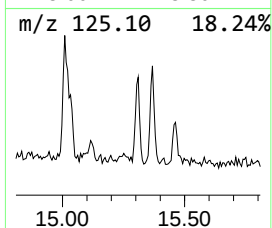
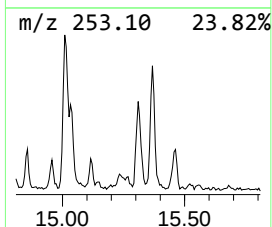
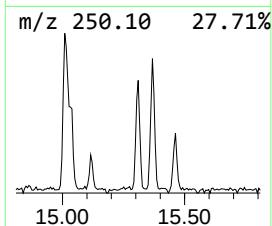
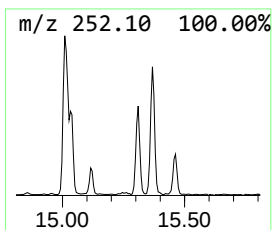
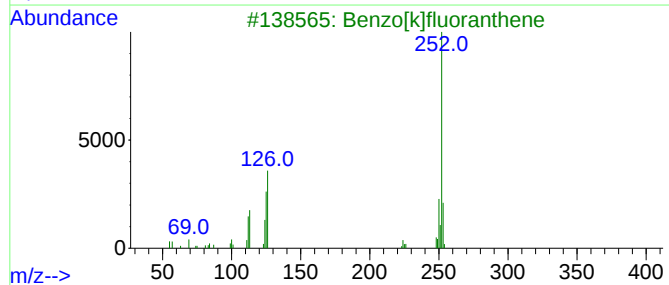
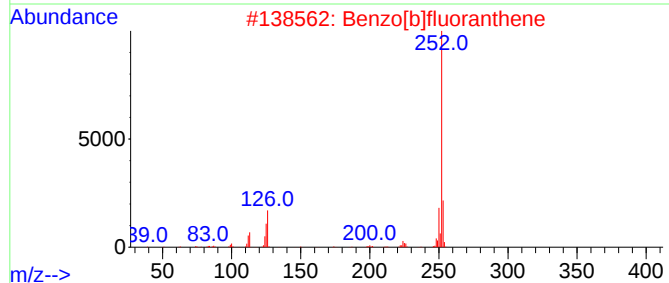
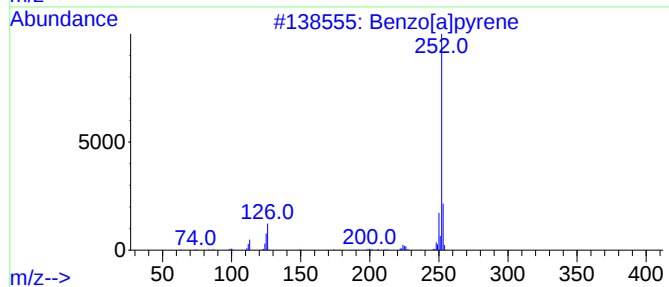
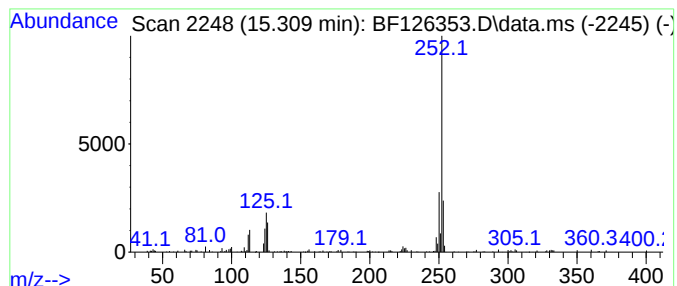
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	6.83 ng	166700	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	94
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[e]pyrene	252	C20H12	000192-97-2	93
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122321\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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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
2-Pentanone, 4-...	5.016	9.1	ng	278217	1	6.816	613369	20.0
Hexadecane	9.257	3.1	ng	109593	3	9.851	700602	20.0
Tritetracontane	9.580	2.1	ng	72443	3	9.851	700602	20.0
Tetradecane	9.792	2.0	ng	71441	3	9.851	700602	20.0
Tris(2-chloropr...	11.204	4.8	ng	172124	4	11.339	717248	20.0
4H-Cyclopenta[d...	11.951	2.7	ng	95604	4	11.339	717248	20.0
unknown12.433	12.433	2.7	ng	95721	4	11.339	717248	20.0
9-Octadecenamid...	13.410	5.5	ng	287268	5	13.980	1047330	20.0
3-Eicosene, (E)-	13.904	8.0	ng	418909	5	13.980	1047330	20.0
Benzo[e]pyrene	15.310	6.8	ng	166700	6	15.433	487870	20.0