

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
 Data File : BF123098.D
 Acq On : 3 Feb 2021 11:58
 Operator : JU/CG
 Sample : M1284-01 5X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-012921

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-BF012721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rBV	113595	146468	6.99%	0.598%
2	5.093	507	511	515	rVB	36329	35779	1.71%	0.146%
3	5.498	576	580	592	rBV	962188	939655	44.86%	3.836%
4	6.504	747	751	770	rBV	1112781	971133	46.36%	3.964%
5	6.892	813	817	820	rBV	1711306	1369795	65.39%	5.591%
6	7.445	902	911	914	rBV	784050	623994	29.79%	2.547%
7	8.175	1030	1035	1038	rBV	2243088	1823768	87.06%	7.444%
8	8.681	1119	1121	1124	rBV3	28931	24838	1.19%	0.101%
9	8.769	1133	1136	1139	rBV3	60623	43593	2.08%	0.178%
10	8.998	1171	1175	1178	rBV2	36812	36820	1.76%	0.150%
11	9.204	1207	1210	1211	rBV2	25287	23798	1.14%	0.097%
12	9.251	1214	1218	1221	rBV	1510146	1174336	56.06%	4.794%
13	9.334	1229	1232	1237	rBV	78107	74328	3.55%	0.303%
14	9.404	1241	1244	1247	rVB	30023	24968	1.19%	0.102%
15	9.510	1260	1262	1268	rVB5	26040	30539	1.46%	0.125%
16	9.616	1278	1280	1282	rVB2	30621	24792	1.18%	0.101%
17	9.645	1282	1285	1289	rBV3	65008	95335	4.55%	0.389%
18	9.716	1293	1297	1299	rVV4	25856	26066	1.24%	0.106%
19	9.869	1320	1323	1328	rVB	88307	74615	3.56%	0.305%
20	9.933	1328	1334	1338	rBV	2443345	2094836	100.00%	8.551%
21	10.128	1360	1367	1374	rBV8	62666	123343	5.89%	0.503%
22	10.228	1381	1384	1386	rVB	35935	26914	1.28%	0.110%
23	10.369	1405	1408	1410	rVB	93966	74082	3.54%	0.302%
24	10.480	1423	1427	1429	rBV3	18222	25718	1.23%	0.105%
25	10.569	1437	1442	1443	rBV2	25855	41003	1.96%	0.167%
26	10.592	1443	1446	1451	rVV	51934	62641	2.99%	0.256%
27	10.639	1451	1454	1458	rVB5	22839	25251	1.21%	0.103%
28	10.722	1464	1468	1472	rBV	781673	718688	34.31%	2.934%
29	10.845	1485	1489	1499	rVB2	92108	163613	7.81%	0.668%
30	11.292	1561	1565	1568	rBV2	79114	85850	4.10%	0.350%
31	11.322	1568	1570	1576	rVB	57935	68159	3.25%	0.278%
32	11.427	1584	1588	1591	rBV	2272572	2085841	99.57%	8.514%
33	11.722	1623	1638	1651	rBV2	305944	1257526	60.03%	5.133%
34	11.822	1651	1655	1657	rVB	238138	189426	9.04%	0.773%
35	11.951	1671	1677	1687	rBV	797518	978788	46.72%	3.995%
36	12.127	1705	1707	1711	rVB	47062	39745	1.90%	0.162%

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Peak Location: TOP

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37	12.510	1764	1772	1773	rBV2	369622	466185	22.25%	1.903%
38	12.533	1773	1776	1783	rVB	1165763	1201958	57.38%	4.906%
39	12.616	1787	1790	1792	rBV	150329	124080	5.92%	0.506%
40	12.639	1792	1794	1796	rVV	69836	61981	2.96%	0.253%
41	12.663	1796	1798	1801	rVB	67427	55414	2.65%	0.226%
42	12.739	1807	1811	1819	rBV	391628	484138	23.11%	1.976%
43	12.874	1831	1834	1836	rBV	53031	50933	2.43%	0.208%
44	13.016	1854	1858	1866	rVB	1531475	1291642	61.66%	5.272%
45	13.251	1896	1898	1905	rVB3	49918	75696	3.61%	0.309%
46	13.504	1933	1941	1950	rVB	252122	581525	27.76%	2.374%
47	13.598	1955	1957	1960	rVB	46252	37942	1.81%	0.155%
48	13.945	2014	2016	2019	rVB	130660	101728	4.86%	0.415%
49	14.074	2034	2038	2042	rVB	1701794	1510116	72.09%	6.164%
50	14.174	2050	2055	2062	rBV	356658	641483	30.62%	2.618%
51	14.551	2117	2119	2122	rVB2	100526	82009	3.91%	0.335%
52	14.733	2146	2150	2155	rVB2	383988	550541	26.28%	2.247%
53	14.863	2170	2172	2175	rVB	101607	90525	4.32%	0.370%
54	15.210	2229	2231	2235	rVB	135160	146923	7.01%	0.600%
55	15.563	2287	2291	2295	rBV	1045431	1317434	62.89%	5.378%

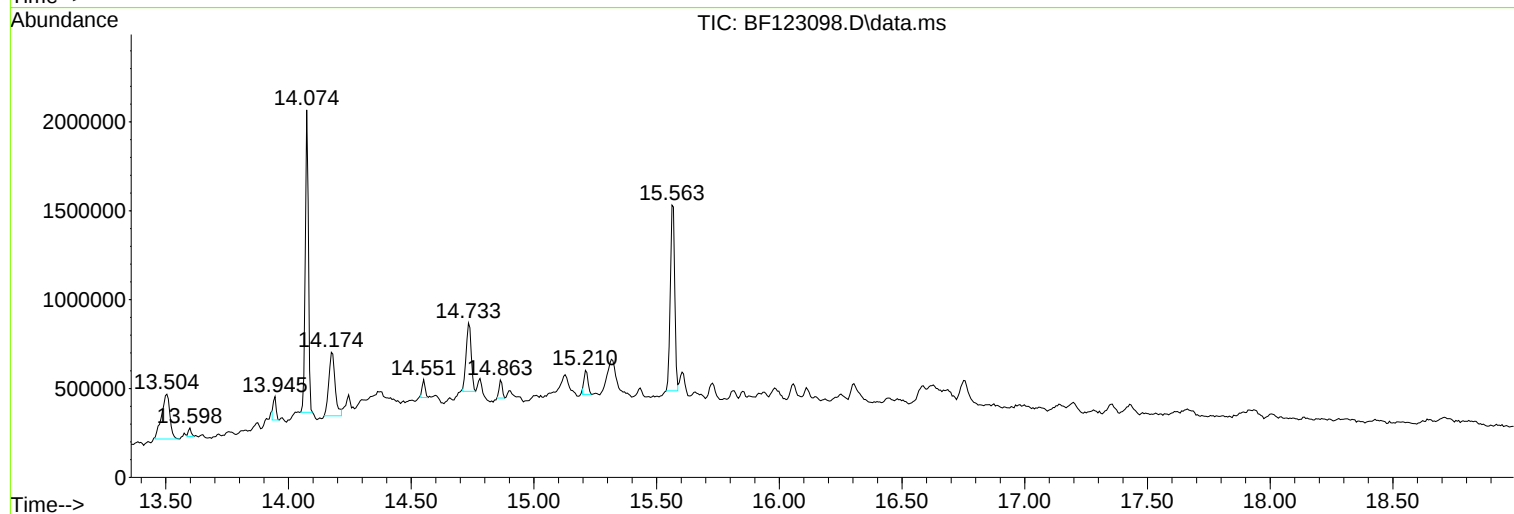
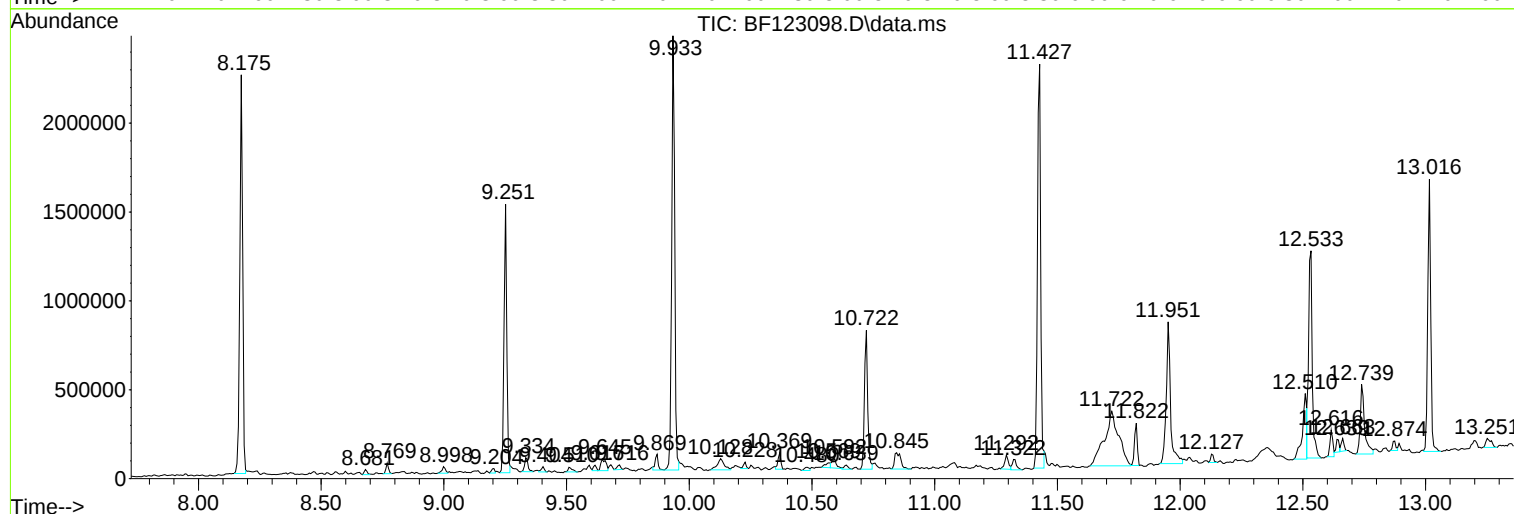
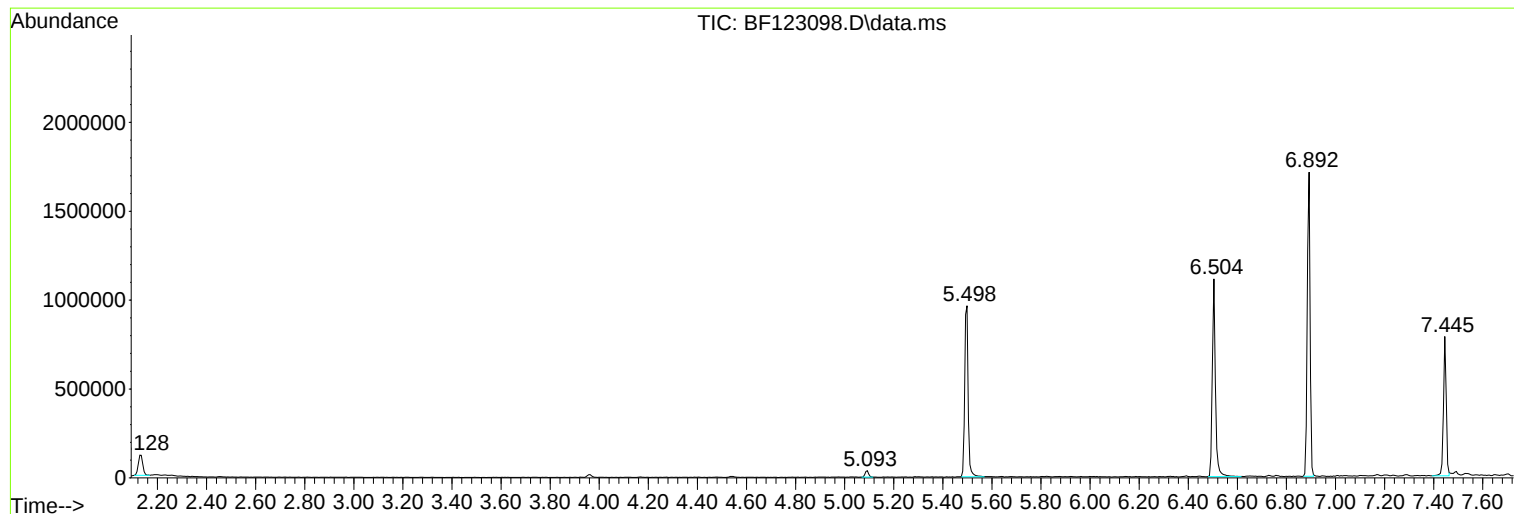
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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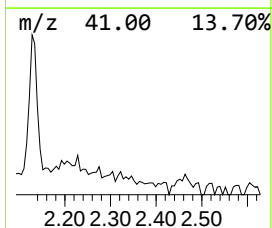
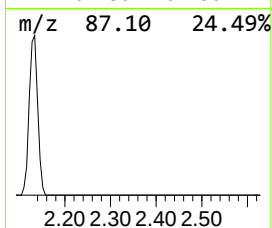
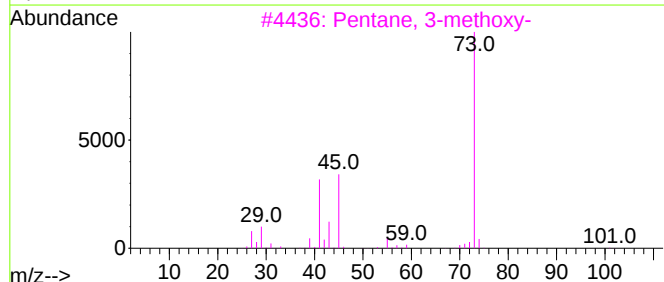
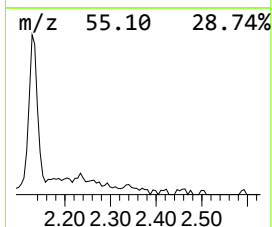
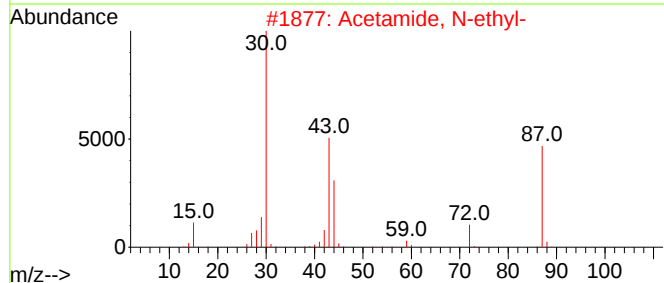
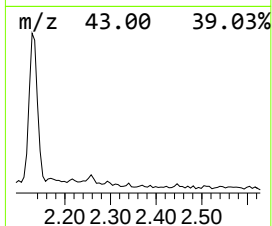
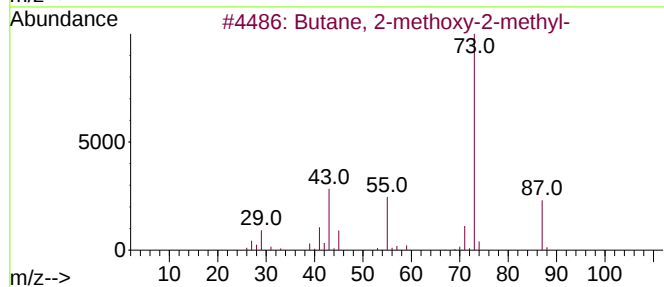
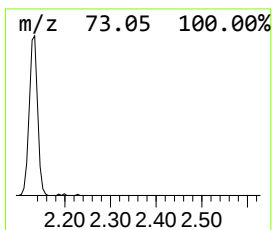
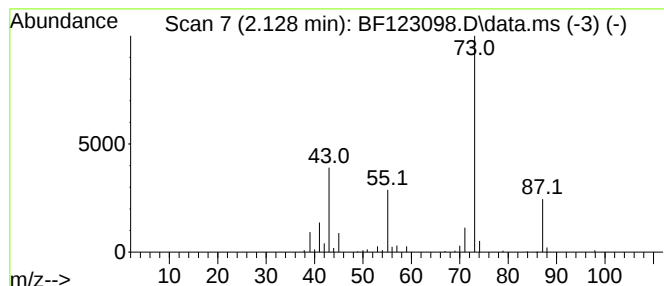
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	2.14 ng	146468	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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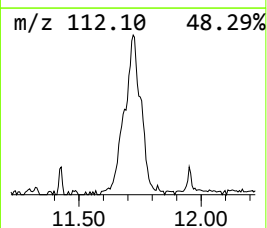
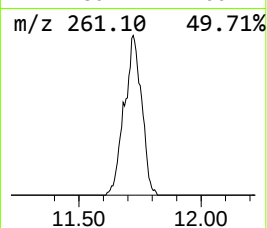
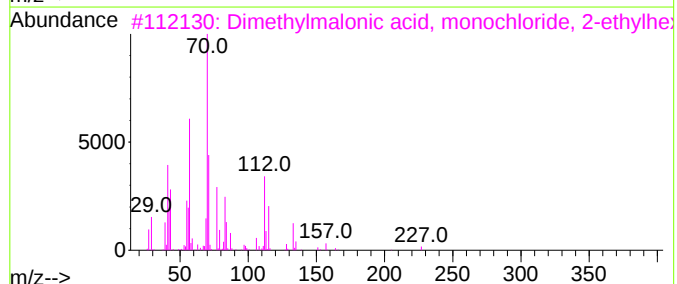
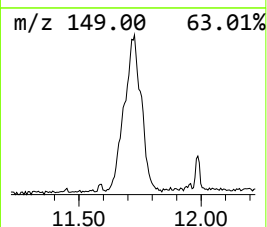
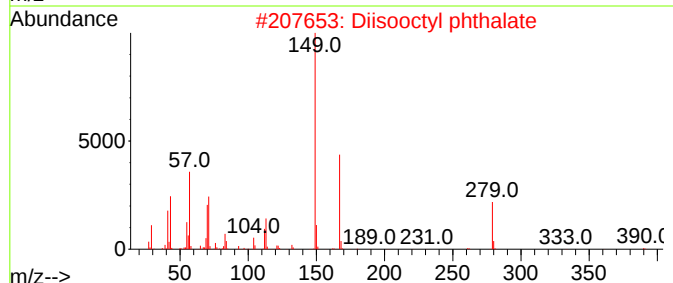
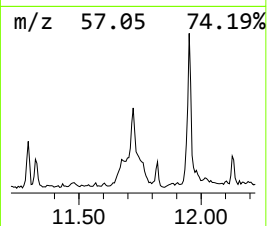
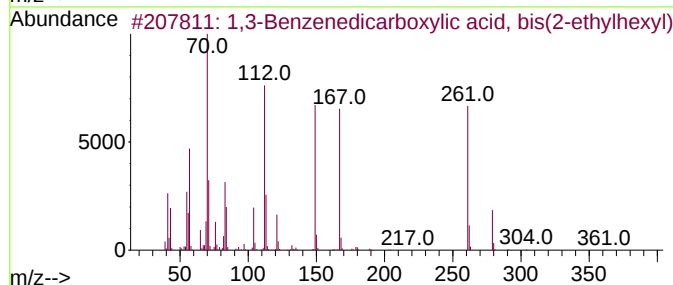
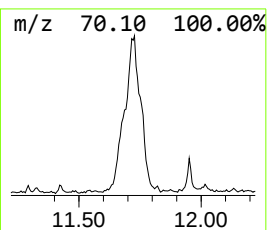
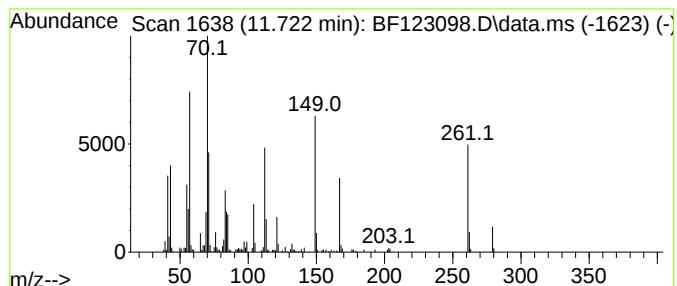
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.722	12.06 ng	1257530	Phenanthrene-d10	11.428	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2	Diisooctyl phthalate	390	C24H38O4	000131-20-4	38
3	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	38
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	35
5	Carbonic acid, allyl 2-ethylhexy...	214	C12H22O3	1000357-80-6	35



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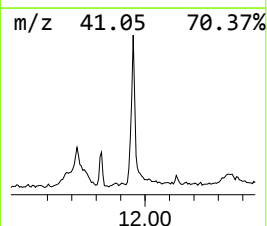
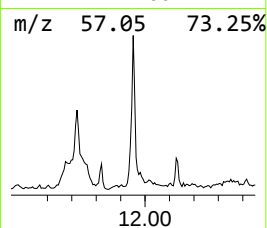
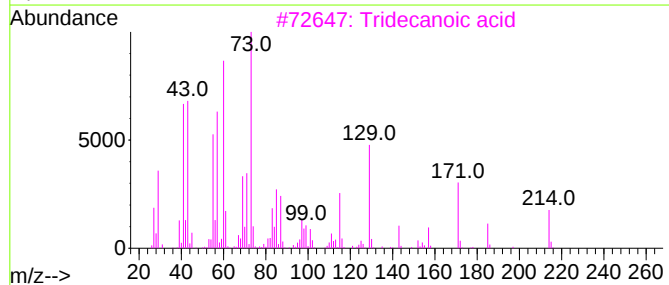
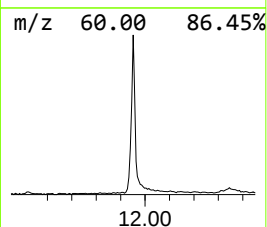
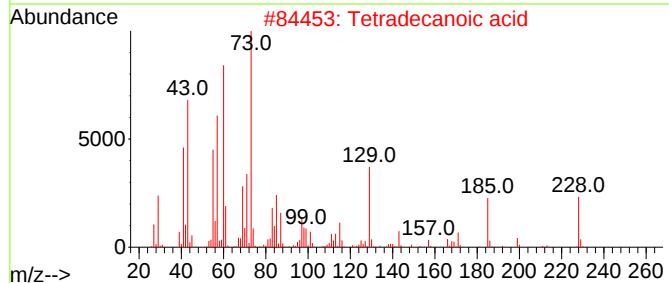
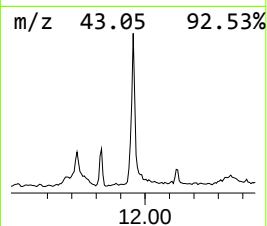
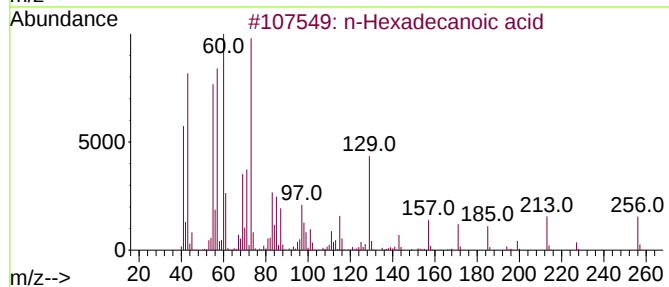
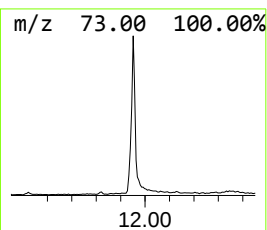
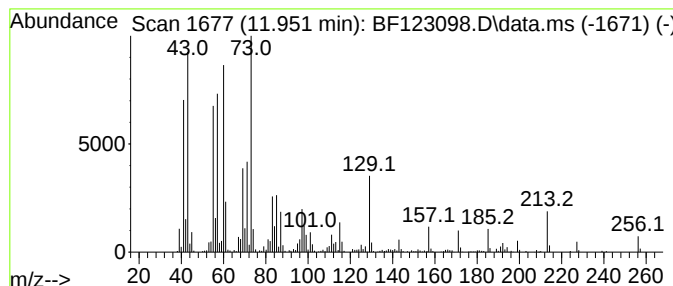
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	9.39 ng	978788	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Estra-1,3,5(10)-trien-17.β-ol	256	C18H24O	002529-64-8	38



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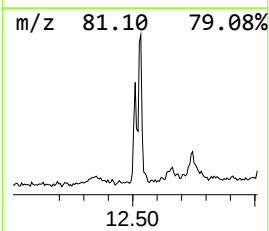
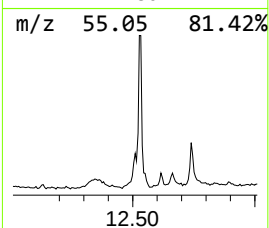
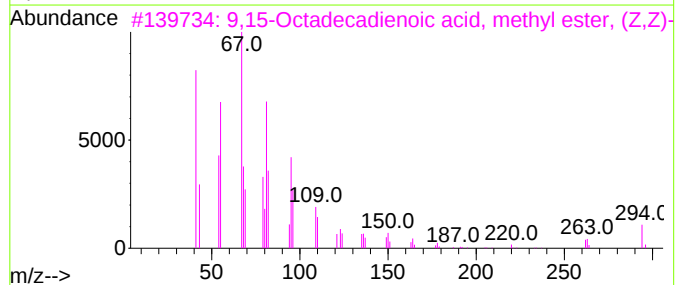
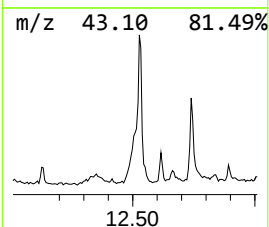
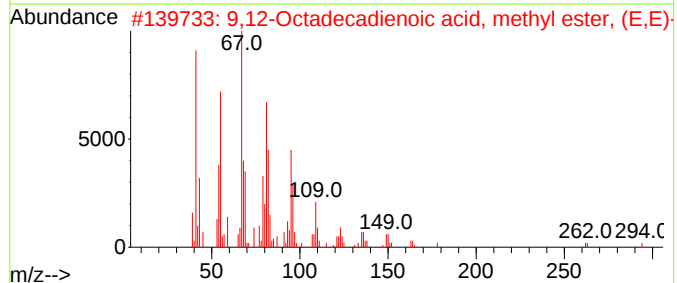
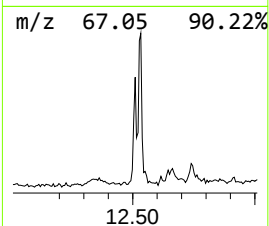
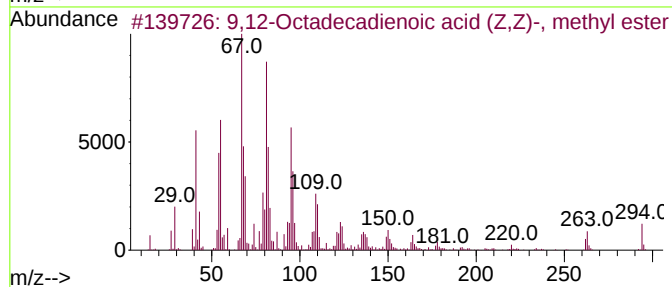
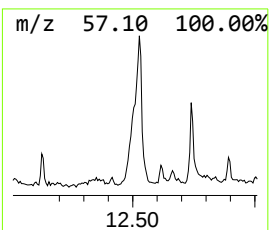
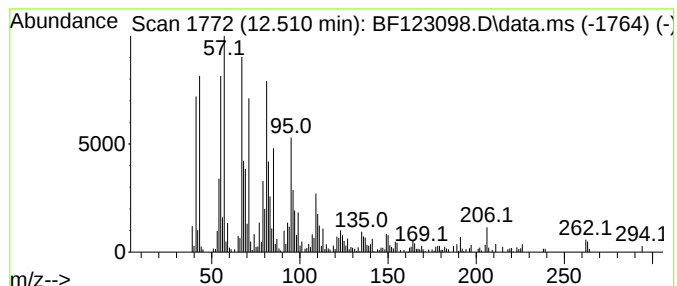
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.510	4.47 ng	466185	Phenanthrene-d10		11.428	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...		294	C19H34O2	000112-63-0	98
2	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	97
3	9,15-Octadecadienoic acid, methy...		294	C19H34O2	017309-05-6	96
4	12,15-Octadecadienoic acid, meth...		294	C19H34O2	057156-97-5	91
5	9,17-Octadecadienal, (Z)-		264	C18H32O	056554-35-9	90



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ALS Vial : 5 Sample Multiplier: 1

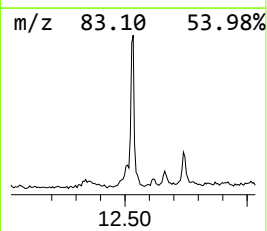
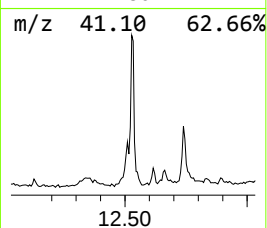
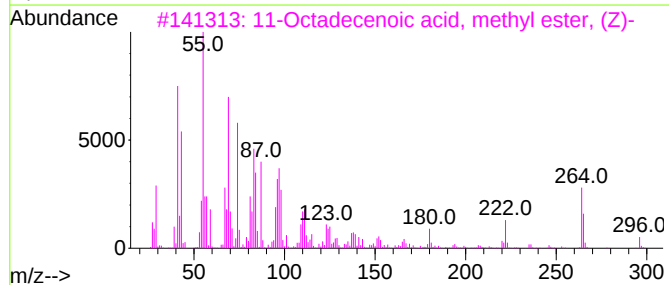
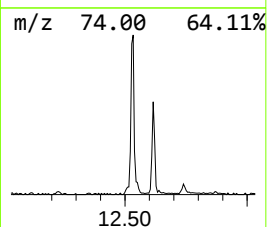
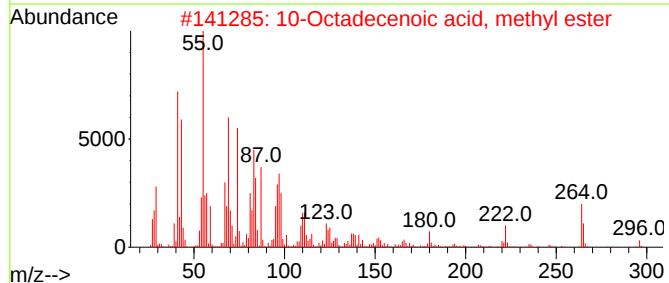
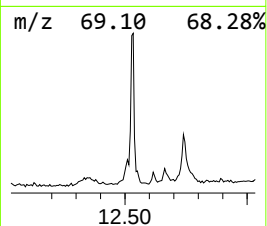
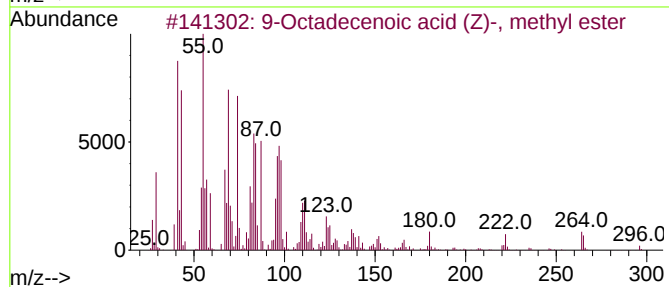
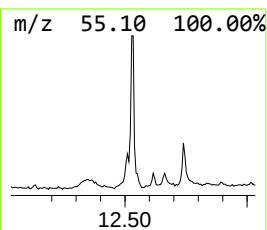
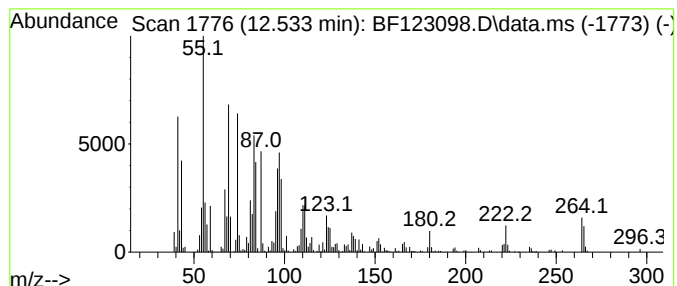
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.533	11.52 ng	1201960	Phenanthrene-d10	11.428	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
Data File : BF123098.D
Acq On : 3 Feb 2021 11:58
Operator : JU/CG
Sample : M1284-01 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-012921

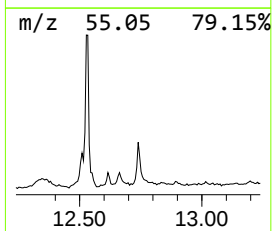
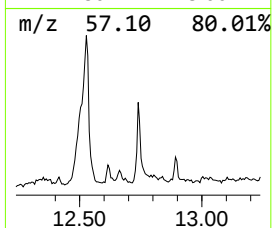
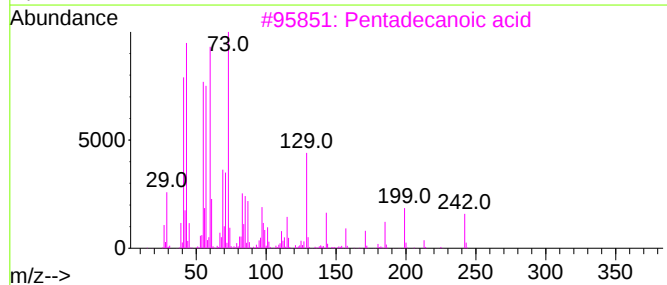
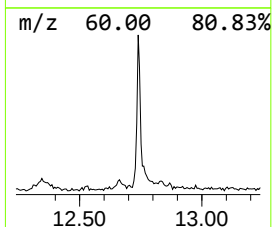
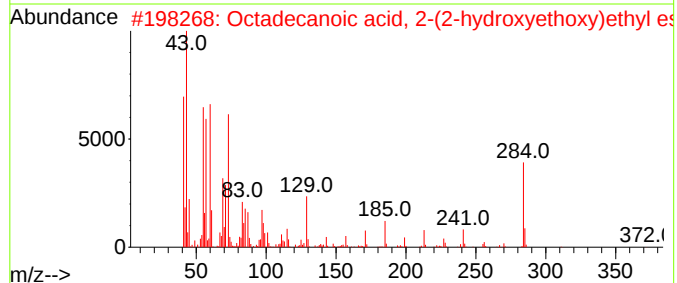
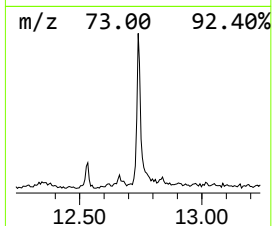
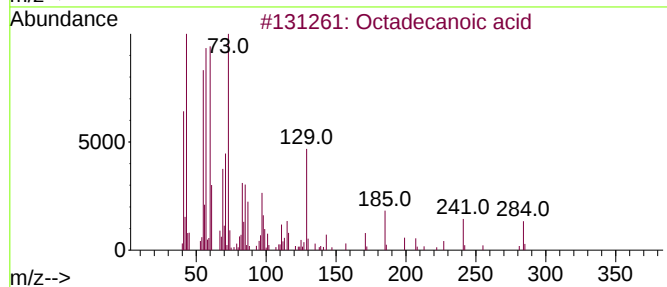
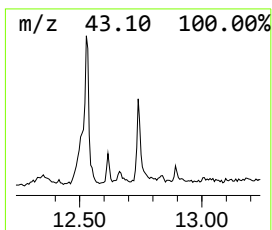
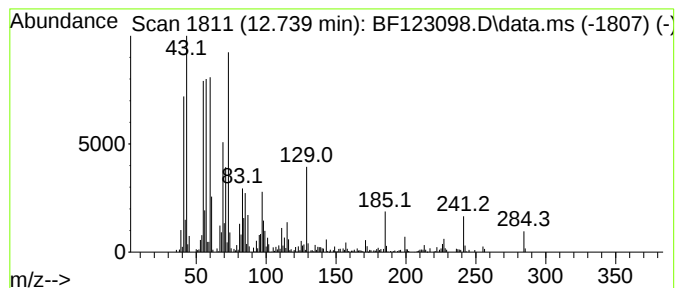
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	4.64 ng	484138	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
Data File : BF123098.D
Acq On : 3 Feb 2021 11:58
Operator : JU/CG
Sample : M1284-01 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-04-012921

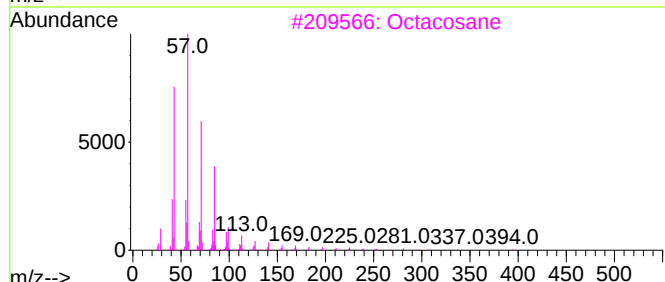
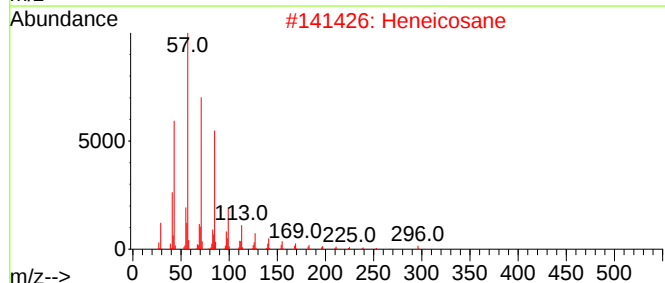
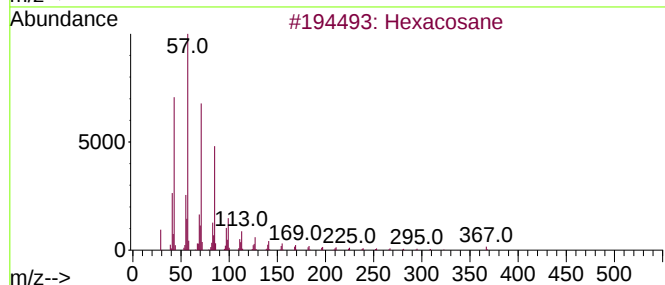
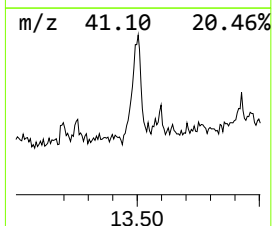
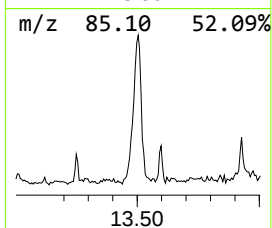
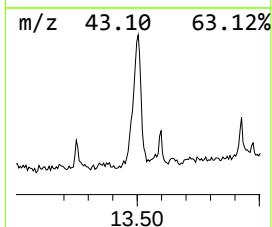
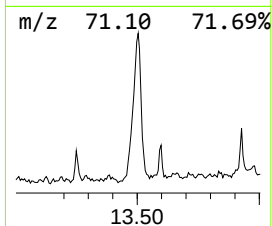
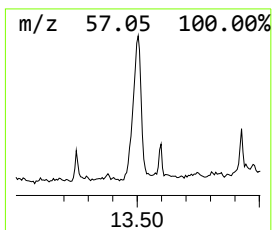
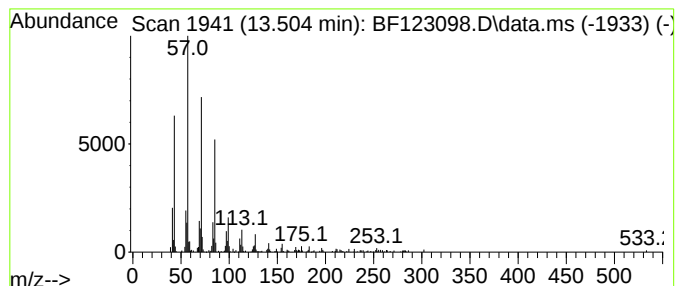
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	7.70 ng	581525	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Tetracosane	338	C24H50	000646-31-1	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
Data File : BF123098.D
Acq On : 3 Feb 2021 11:58
Operator : JU/CG
Sample : M1284-01 5X
Misc :
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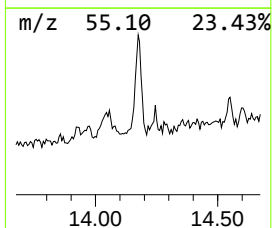
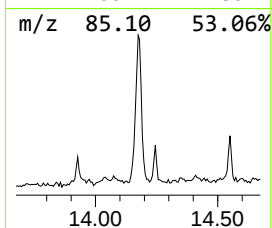
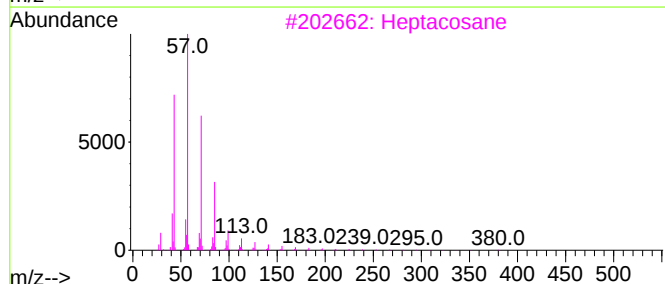
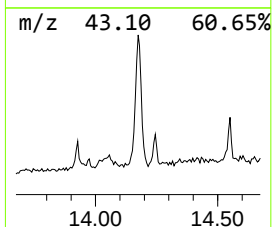
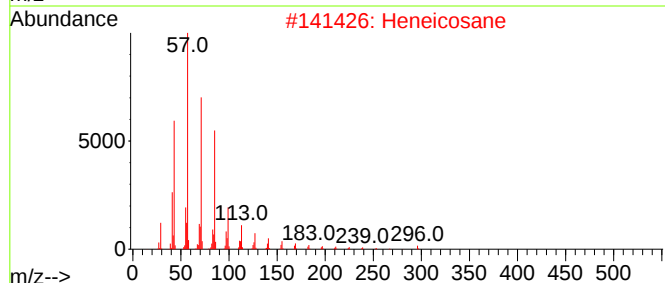
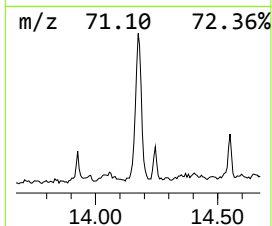
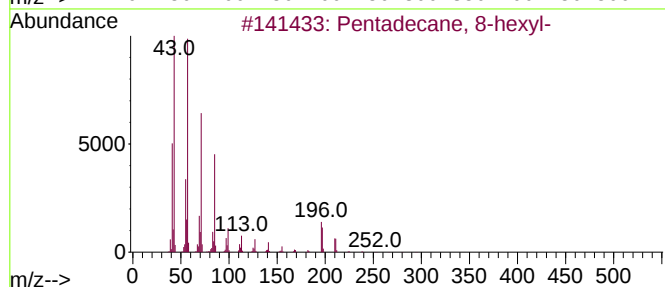
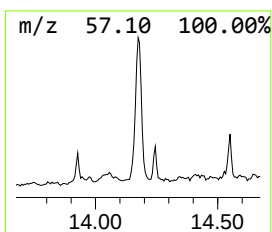
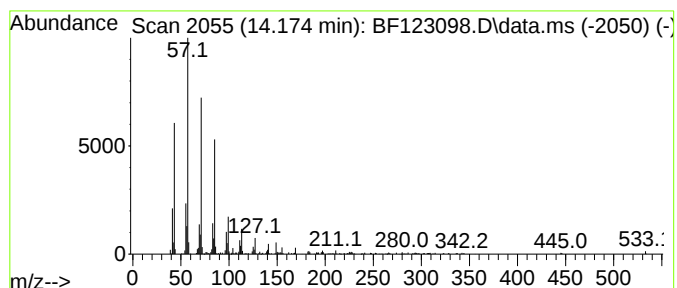
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.174	8.50 ng	641483	Chrysene-d12	14.074	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
Data File : BF123098.D
Acq On : 3 Feb 2021 11:58
Operator : JU/CG
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Misc :
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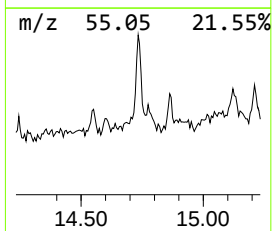
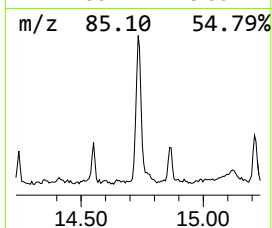
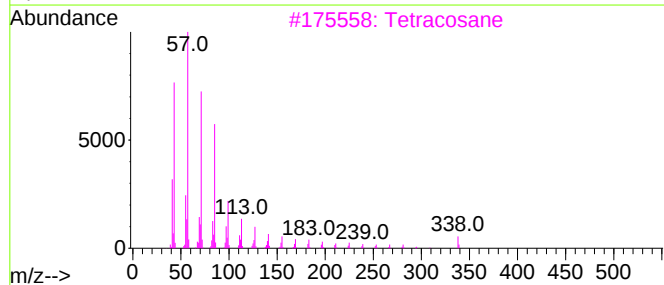
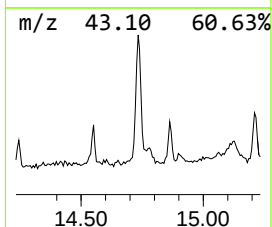
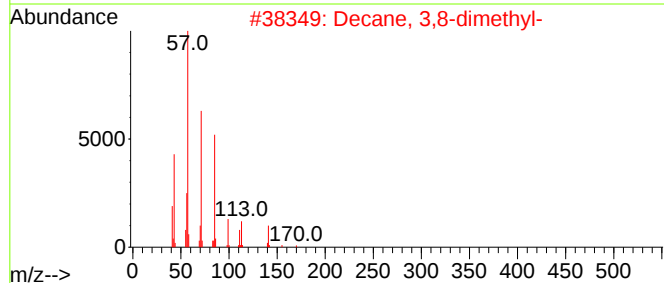
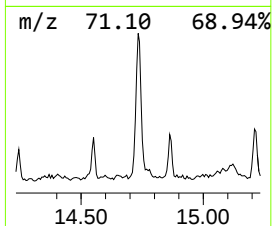
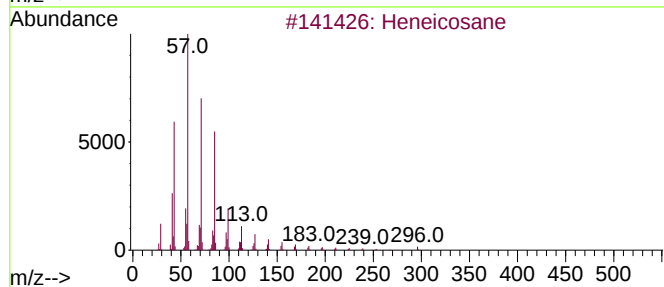
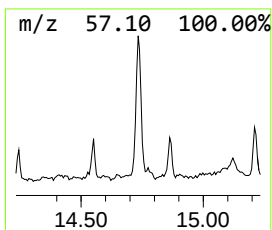
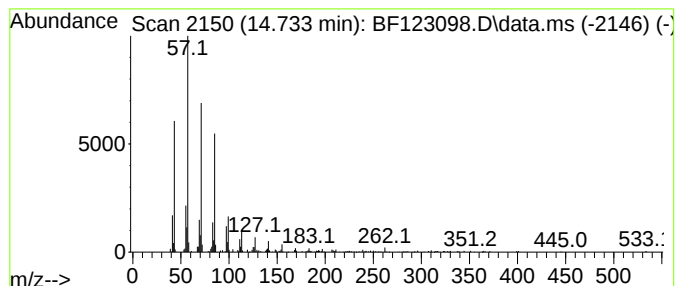
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	7.29 ng	550541	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3			Tetracosane	338	C24H50	000646-31-1	87
4			Docosane, 11-butyl-	366	C26H54	013475-76-8	86
5			Tetratetracontane	619	C44H90	007098-22-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
Data File : BF123098.D
Acq On : 3 Feb 2021 11:58
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-04-012921

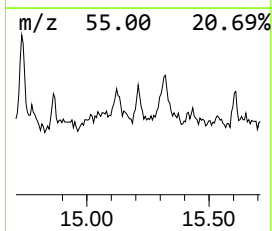
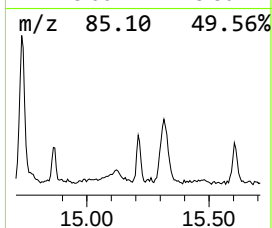
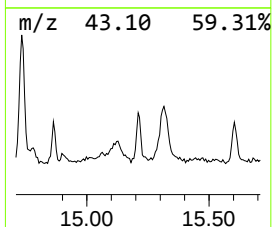
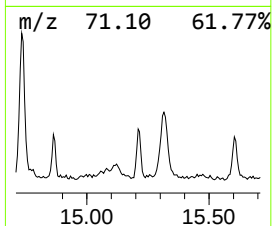
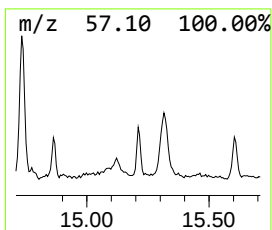
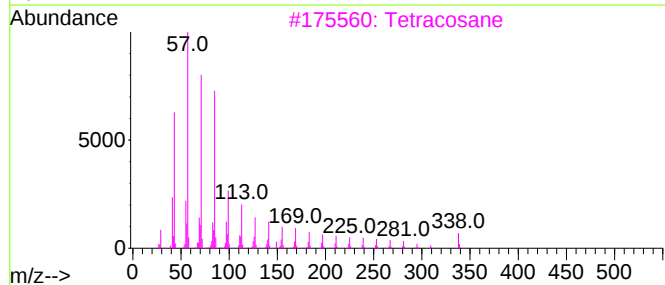
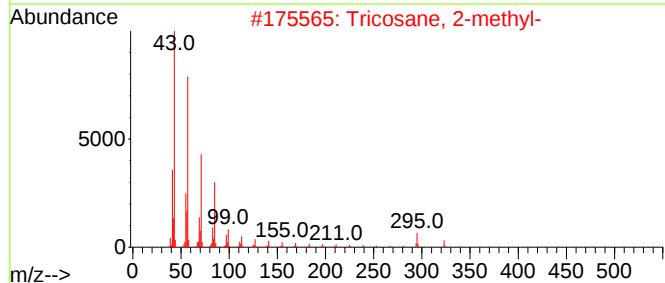
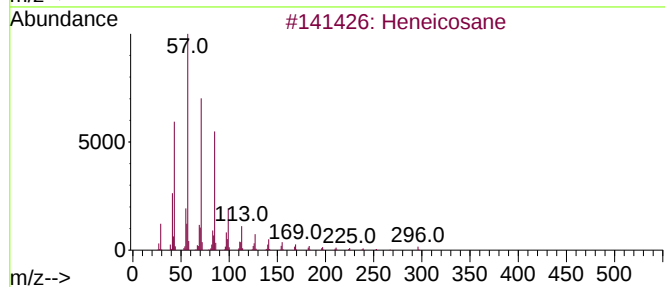
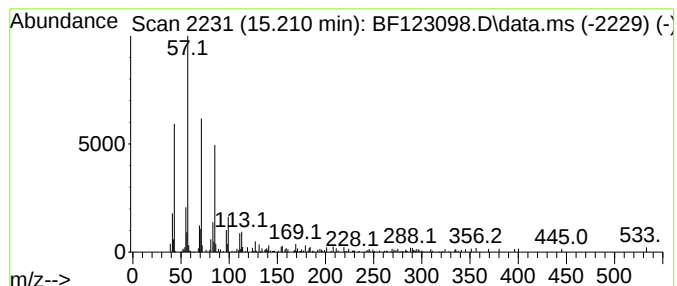
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tricosane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	2.23 ng	146923	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	93
2			Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heptacosane	380	C27H56	000593-49-7	90
5			Tricosane	324	C23H48	000638-67-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020321\
Data File : BF123098.D
Acq On : 3 Feb 2021 11:58
Operator : JU/CG
Sample : M1284-01 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

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

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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1,3-Benzenedica...	11.722	12.1	ng	1257530	4	11.428	2085840	20.0
n-Hexadecanoic ...	11.951	9.4	ng	978788	4	11.428	2085840	20.0
9,12-Octadecadi...	12.510	4.5	ng	466185	4	11.428	2085840	20.0
9-Octadecenoic ...	12.533	11.5	ng	1201960	4	11.428	2085840	20.0
Octadecanoic acid	12.739	4.6	ng	484138	4	11.428	2085840	20.0
Hexacosane	13.504	7.7	ng	581525	5	14.074	1510120	20.0
Pentadecane, 8-...	14.174	8.5	ng	641483	5	14.074	1510120	20.0
Heneicosane	14.733	7.3	ng	550541	5	14.074	1510120	20.0
Tricosane, 2-me...	15.210	2.2	ng	146923	6	15.568	1317430	20.0