

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031318\
 Data File : BF103607.D
 Acq On : 13 Mar 2018 16:35
 Operator : SJ/JU
 Sample : J1753-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.092	508	511	520	rBV	22366	52815	1.71%	0.171%
2	5.481	574	577	607	rBV	843411	2494616	80.71%	8.082%
3	6.498	747	750	769	rBV	1231929	2775638	89.81%	8.992%
4	6.628	769	772	800	rVB	1939058	2990872	96.77%	9.689%
5	6.857	808	811	833	rVB	474279	851297	27.54%	2.758%
6	7.010	833	837	866	rVB	1611040	2064592	66.80%	6.689%
7	7.428	904	908	932	rBV	1025948	1941769	62.83%	6.291%
8	8.139	1026	1029	1055	rBV	682278	1162874	37.63%	3.767%
9	9.016	1175	1178	1180	rBV	32278	32221	1.04%	0.104%
10	9.075	1185	1188	1197	rVB	156159	150145	4.86%	0.486%
11	9.186	1204	1207	1208	rBV	145963	115575	3.74%	0.374%
12	9.210	1208	1211	1226	rVV	2585602	3090686	100.00%	10.013%
13	9.316	1226	1229	1239	rVB3	46933	76981	2.49%	0.249%
14	9.398	1239	1243	1256	rBV2	59214	171899	5.56%	0.557%
15	9.692	1290	1293	1300	rBV2	24285	33408	1.08%	0.108%
16	9.898	1324	1328	1341	rBV	1125586	1235685	39.98%	4.003%
17	10.280	1389	1393	1396	rBV	63684	57605	1.86%	0.187%
18	10.310	1396	1398	1401	rVB	42363	37649	1.22%	0.122%
19	10.698	1460	1464	1476	rBV	1352338	1967414	63.66%	6.374%
20	10.780	1476	1478	1484	rVB2	39997	56460	1.83%	0.183%
21	10.886	1492	1496	1500	rBV2	31802	35921	1.16%	0.116%
22	11.227	1551	1554	1557	rBV2	34124	41550	1.34%	0.135%
23	11.398	1579	1583	1597	rBV	964431	1324761	42.86%	4.292%
24	11.539	1604	1607	1610	rBV	220755	189513	6.13%	0.614%
25	11.598	1613	1617	1624	rVB4	48390	70345	2.28%	0.228%
26	11.657	1624	1627	1629	rBV	52765	41564	1.34%	0.135%
27	11.910	1666	1670	1672	rVV	615455	559927	18.12%	1.814%
28	11.939	1672	1675	1685	rVB	1167168	1179818	38.17%	3.822%
29	12.063	1694	1696	1699	rBV	44124	37133	1.20%	0.120%
30	12.145	1705	1710	1713	rBV4	37234	40160	1.30%	0.130%
31	12.416	1753	1756	1760	rBV	34482	36480	1.18%	0.118%
32	12.451	1760	1762	1765	rVV	73250	63051	2.04%	0.204%
33	12.539	1775	1777	1783	rVB4	24112	34971	1.13%	0.113%
34	12.692	1800	1803	1807	rBV2	58312	67642	2.19%	0.219%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

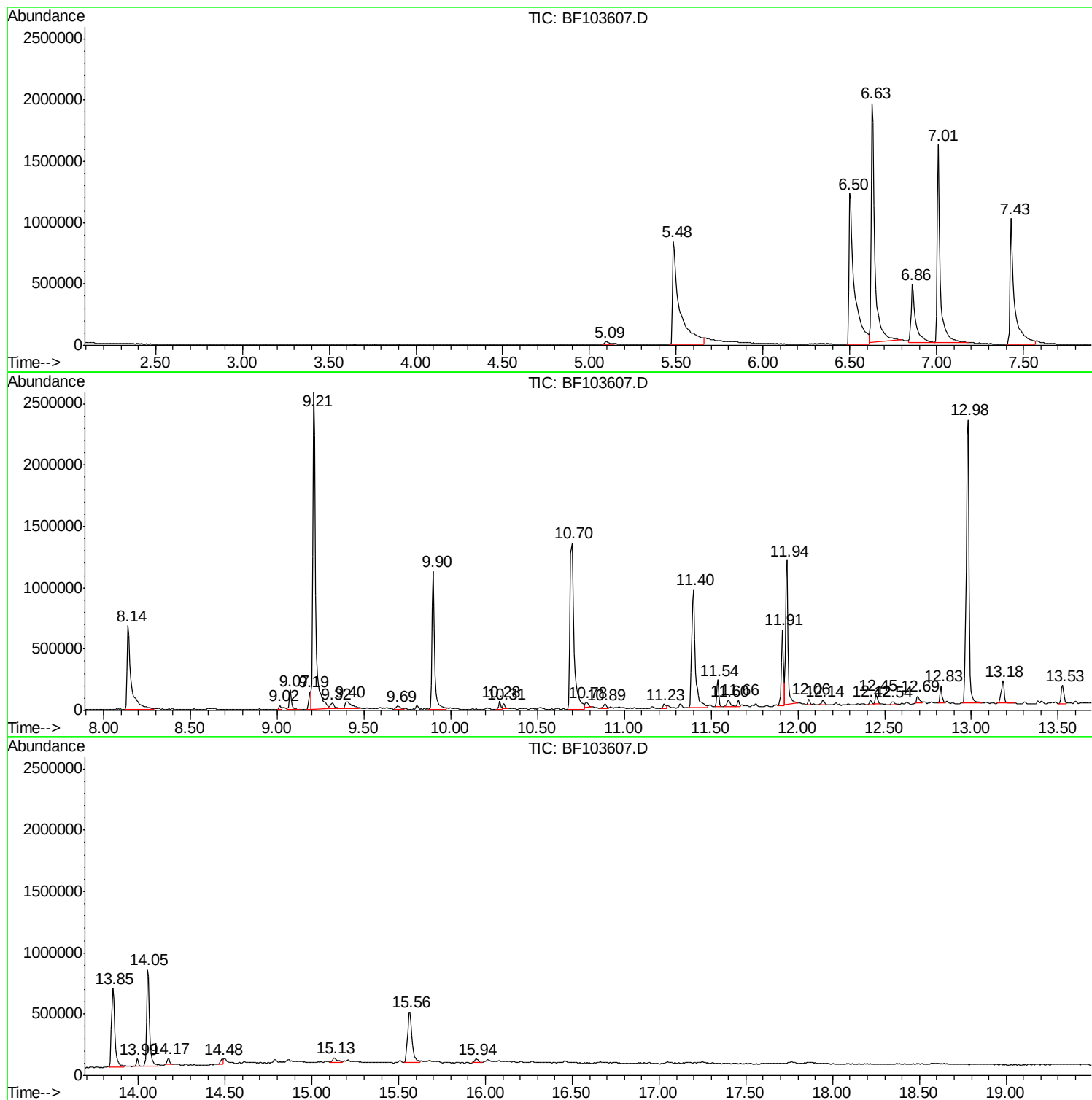
35	12.827	1823	1826	1829	rBV	139700	110766	3.58%	0.359%
36	12.980	1847	1852	1865	rBV	2312178	2562306	82.90%	8.301%
37	13.180	1881	1886	1897	rBV	185449	243835	7.89%	0.790%
38	13.527	1941	1945	1948	rBV	146199	138934	4.50%	0.450%
39	13.851	1997	2000	2011	rBV	642614	774600	25.06%	2.509%
40	13.992	2021	2024	2027	rVB	60519	51816	1.68%	0.168%
41	14.051	2031	2034	2044	rBV	783076	955664	30.92%	3.096%
42	14.174	2052	2055	2059	rBV2	48984	50500	1.63%	0.164%
43	14.480	2104	2107	2108	rBV	39687	35637	1.15%	0.115%
44	15.127	2214	2217	2225	rBV3	38271	65138	2.11%	0.211%
45	15.562	2286	2291	2301	rBV	416482	747398	24.18%	2.421%
46	15.945	2353	2356	2362	rBV3	32440	47675	1.54%	0.154%

Sum of corrected areas: 30867306

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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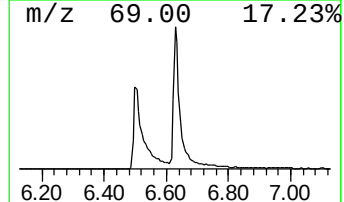
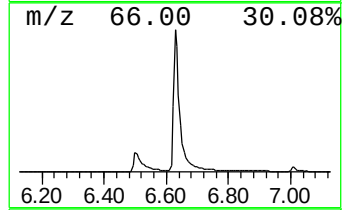
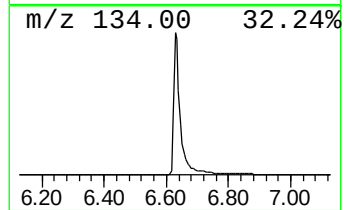
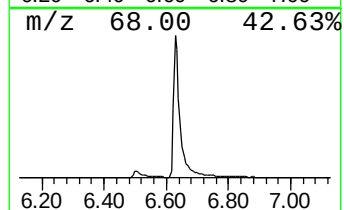
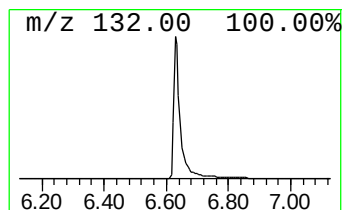
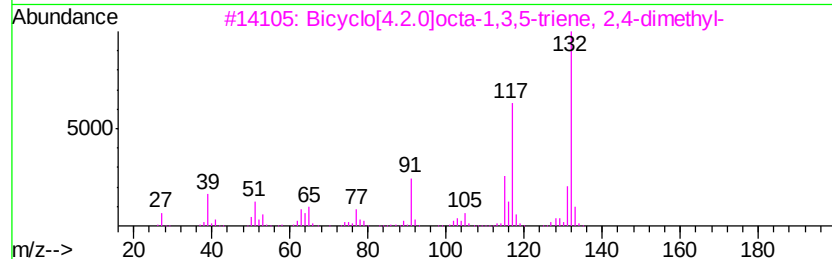
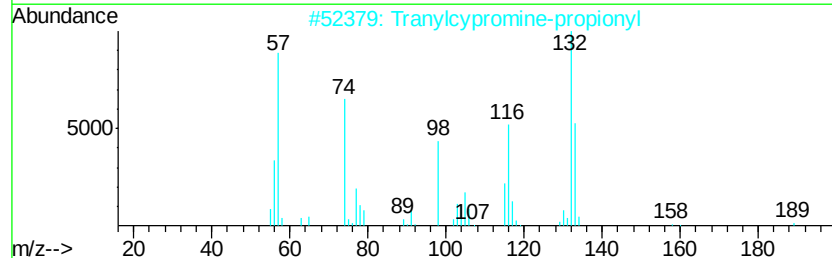
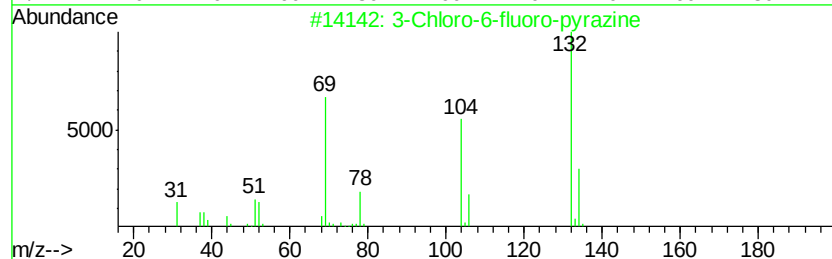
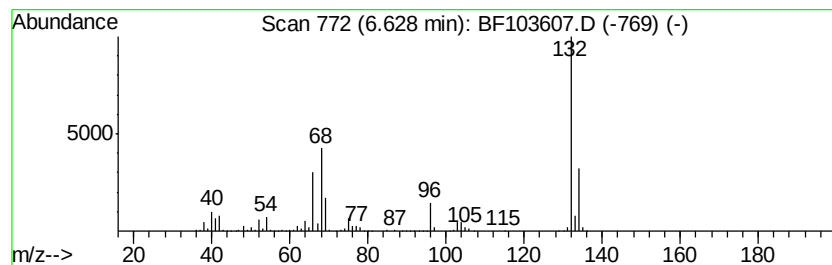
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	70.27 ng	2990870	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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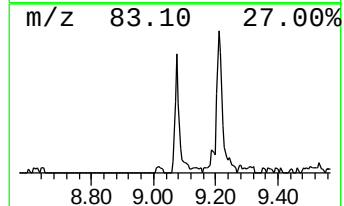
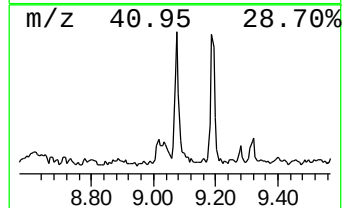
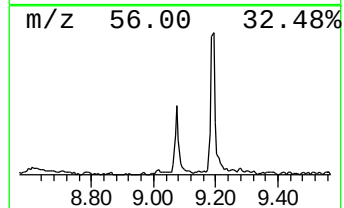
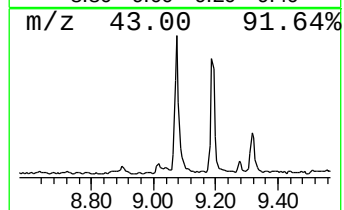
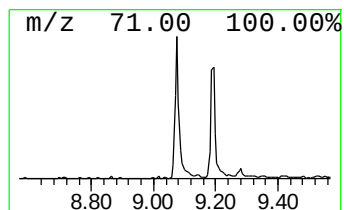
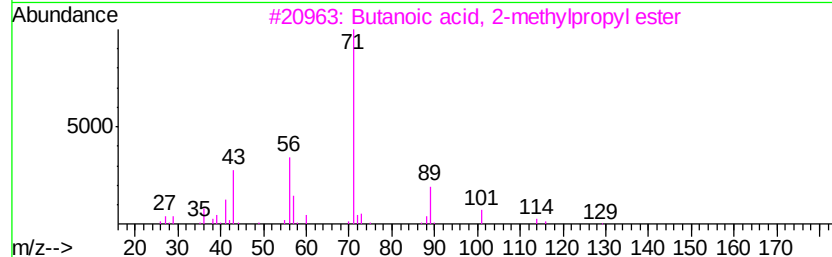
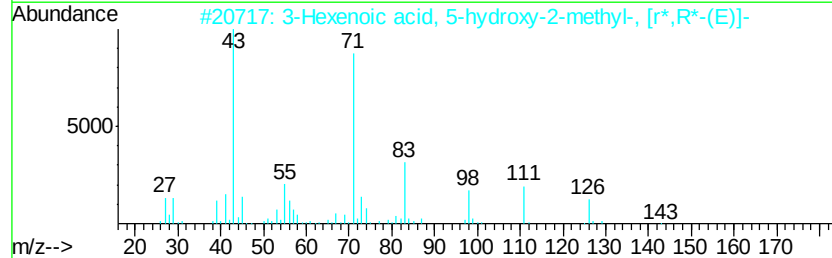
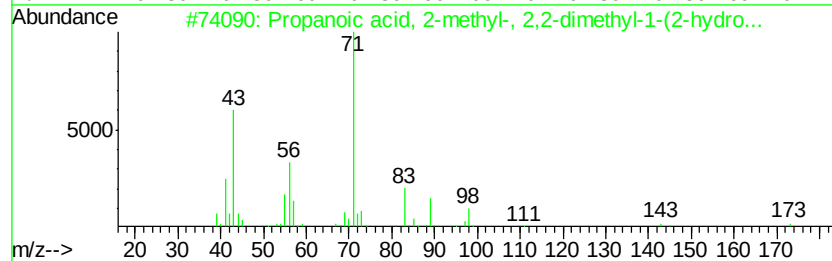
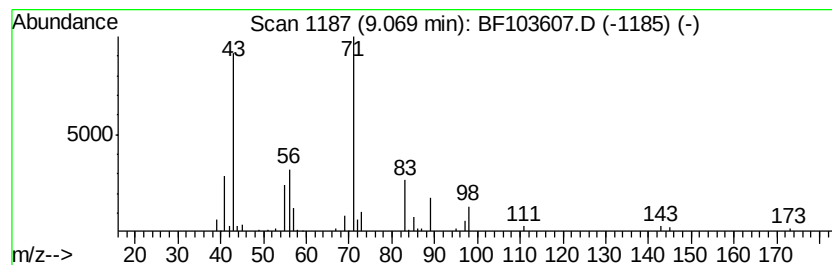
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	2.43 ng	150145	Acenaphthene-d10	9.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	74
2		3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	45
3		Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40
4		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40
5		2,5-Dimethyl-1,5-hexadien-3-ol	126	C8H14O	017123-63-6	38



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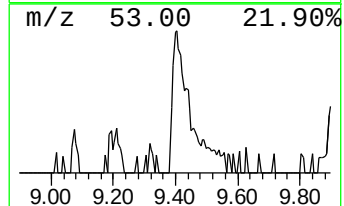
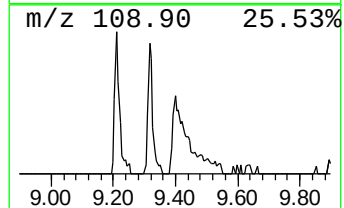
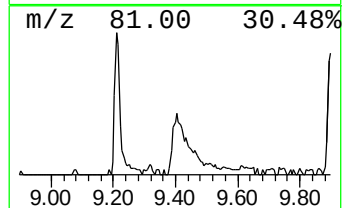
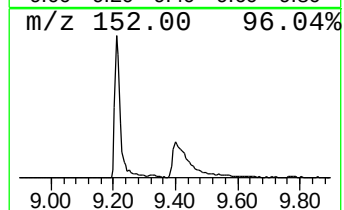
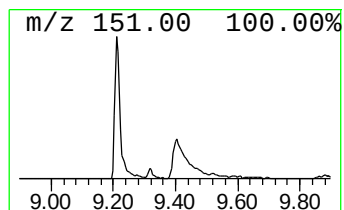
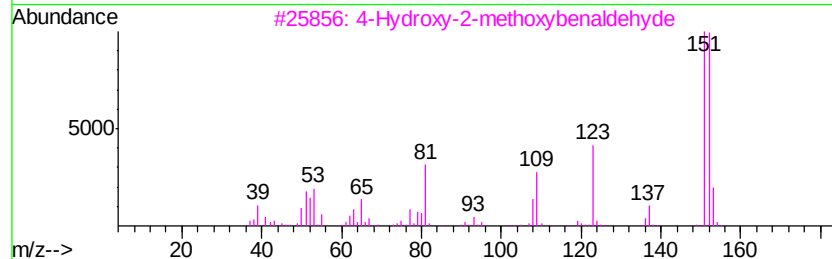
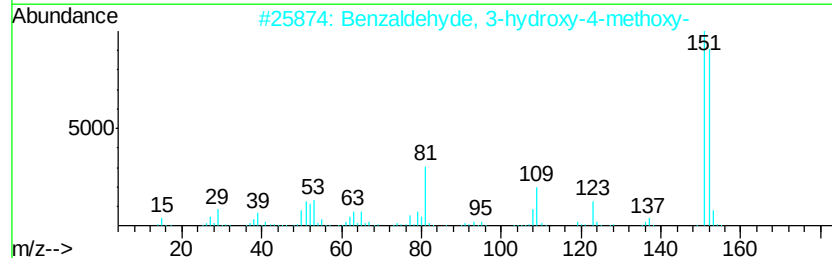
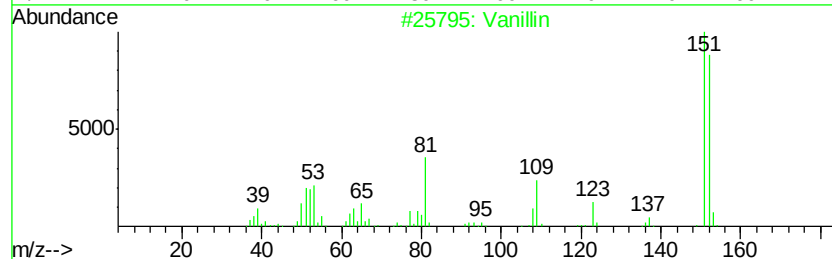
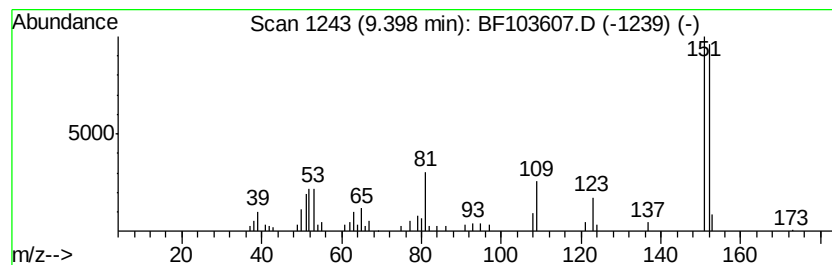
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Vanillin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.40	2.78 ng	171899	Acenaphthene-d10	9.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin		152	C8H8O3	000121-33-5	96
2	Benzaldehyde, 3-hydroxy-4-methoxy-		152	C8H8O3	000621-59-0	94
3	4-Hydroxy-2-methoxybenaldehyde		152	C8H8O3	018278-34-7	70
4	2-Methyl-6-nitroaniline		152	C7H8N2O2	000570-24-1	43
5	Benzaldehyde, 2,4-dihydroxy-6-me...		152	C8H8O3	000487-69-4	43



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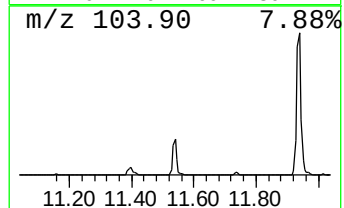
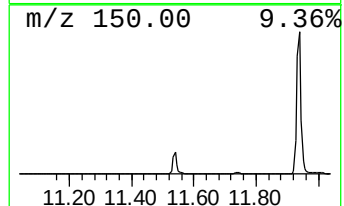
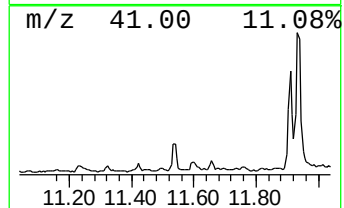
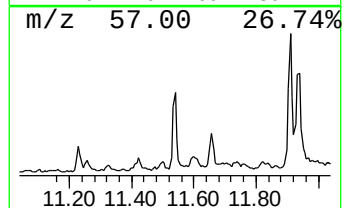
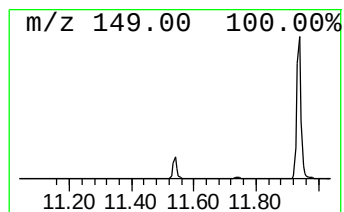
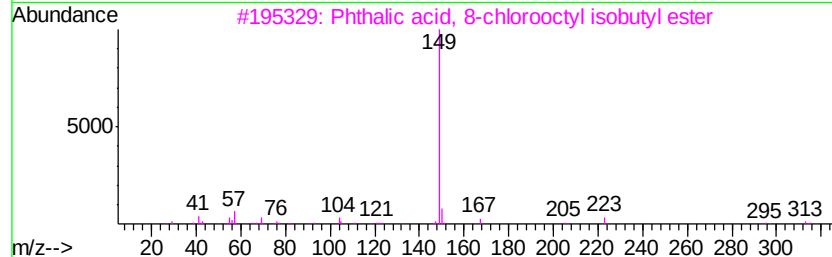
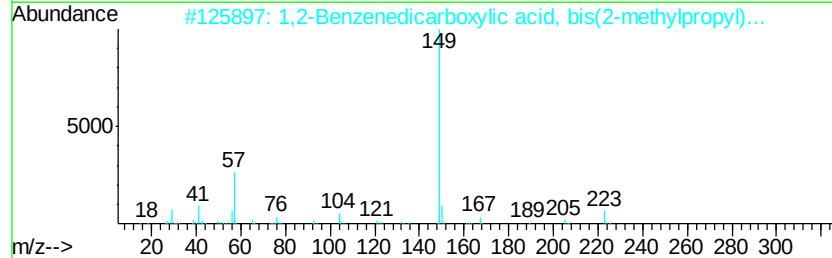
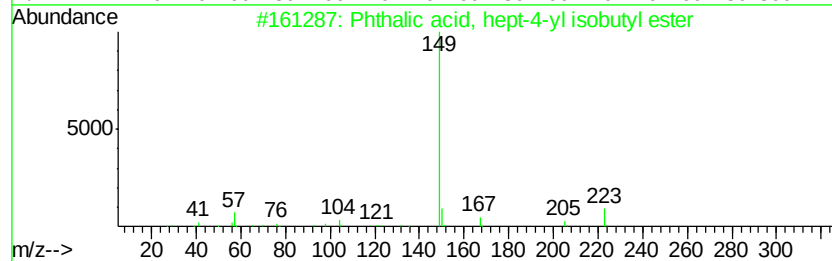
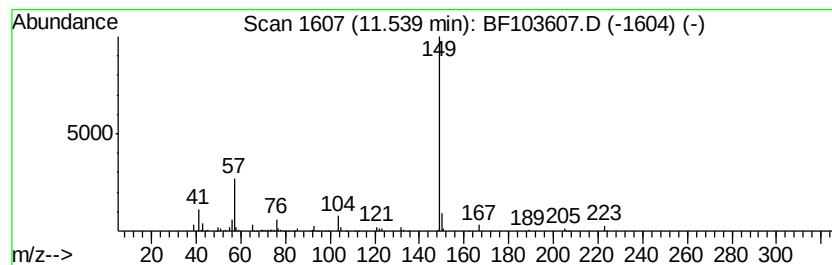
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phthalic acid, hept-4-yl is... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.86 ng	189513	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hept-4-yl isobuty...	320	C19H28O4	1000356-78-3	90
2		1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	86
3		Phthalic acid, 8-chlorooctyl iso...	368	C20H29ClO4	1000356-85-8	83
4		Phthalic acid, decyl isobutyl ester	362	C22H34O4	1000308-94-2	83
5		Phthalic acid, 5-methylhex-2-yl ...	320	C19H28O4	1000371-09-1	83



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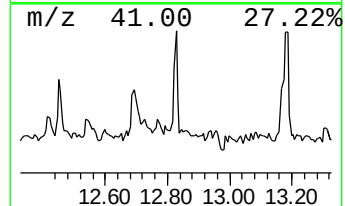
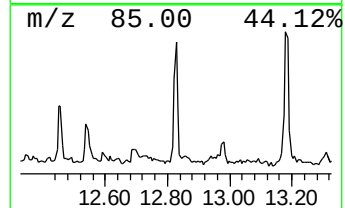
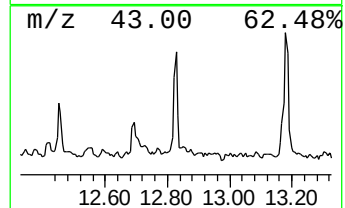
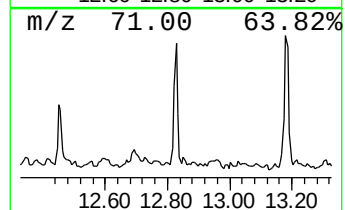
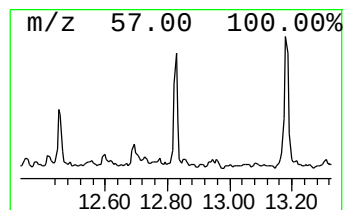
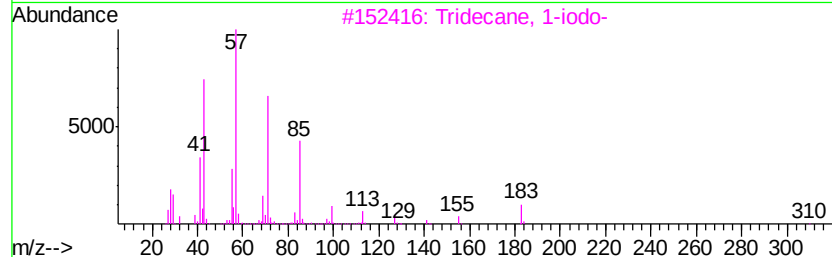
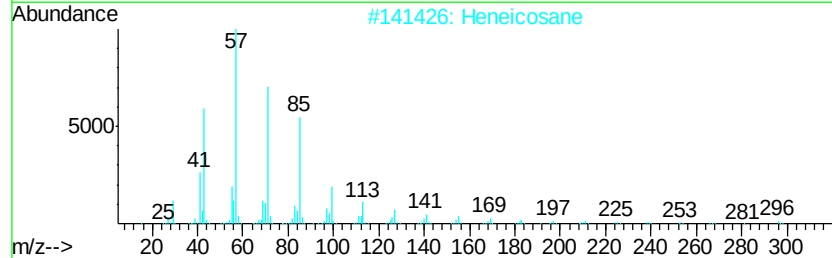
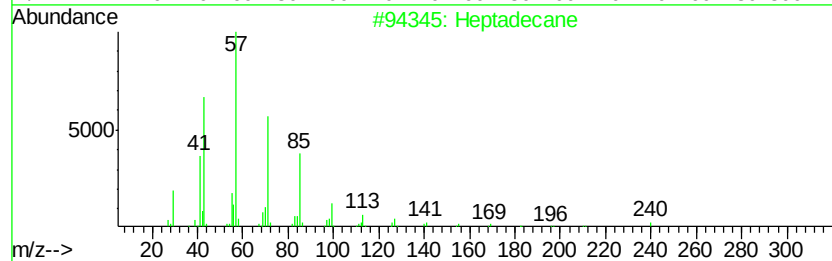
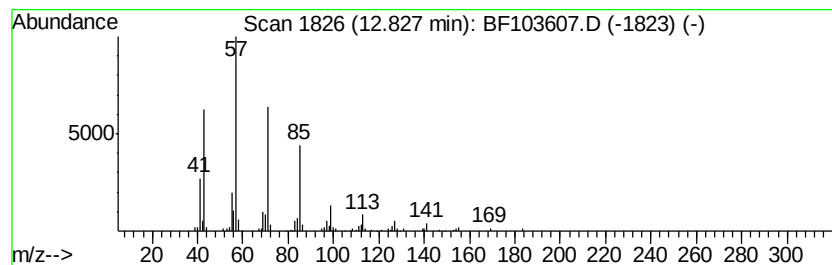
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.32 ng	110766	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



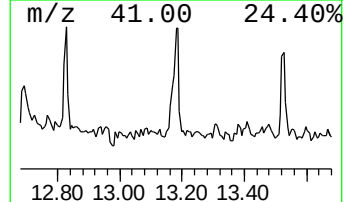
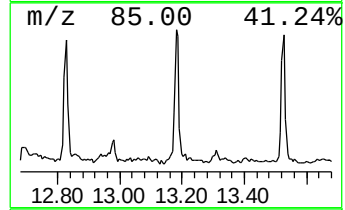
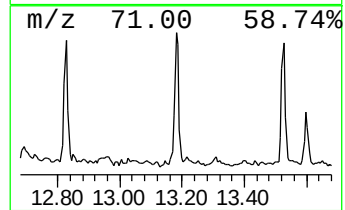
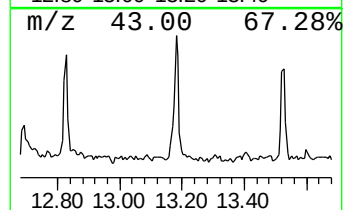
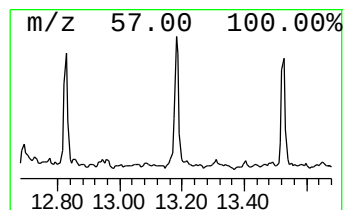
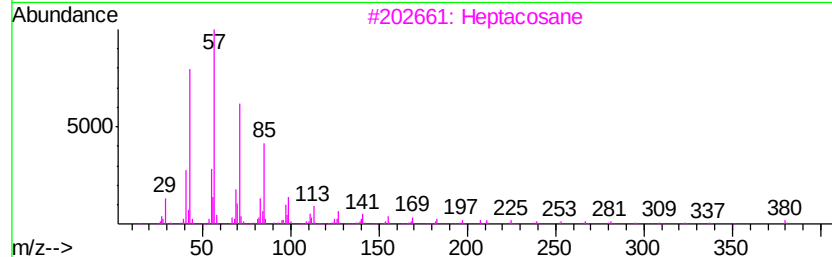
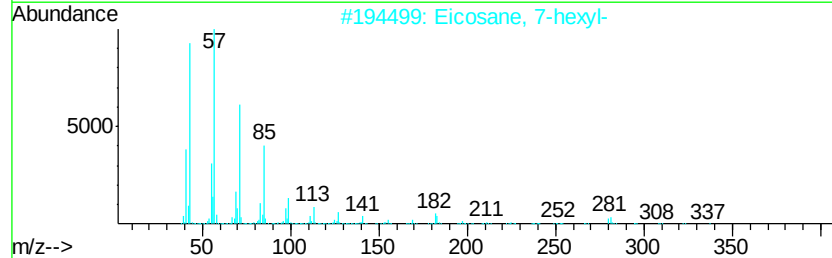
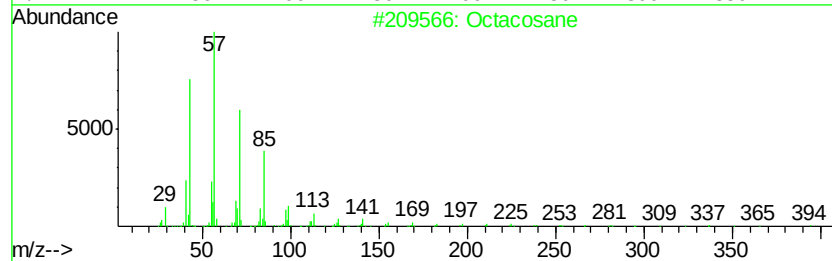
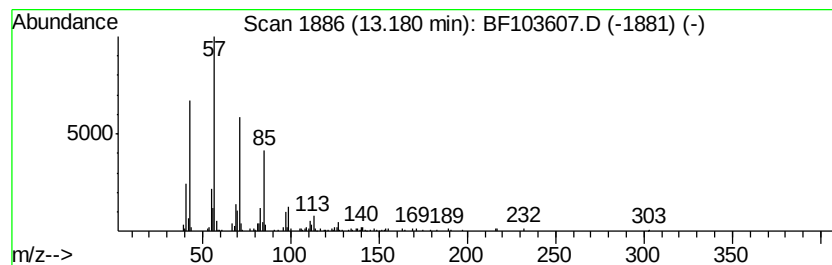
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Acq On : 13 Mar 2018 16:35
Operator : SJ/JU
Sample : J1753-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.18	5.10 ng	243835	Chrysene-d12		14.05
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Hexatriacontane	507	C36H74	000630-06-8	86
5	Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
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Acq On : 13 Mar 2018 16:35
Operator : SJ/JU
Sample : J1753-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

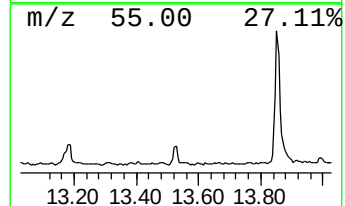
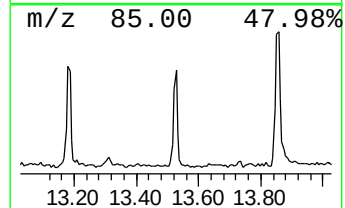
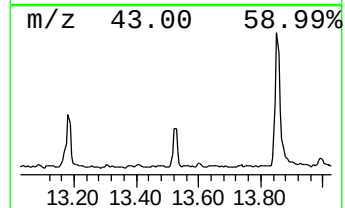
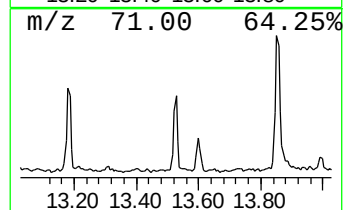
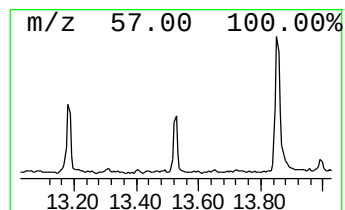
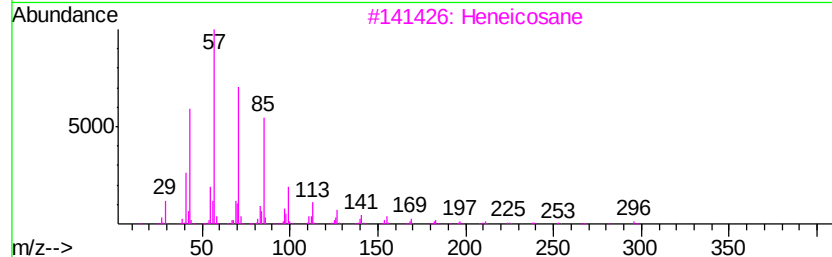
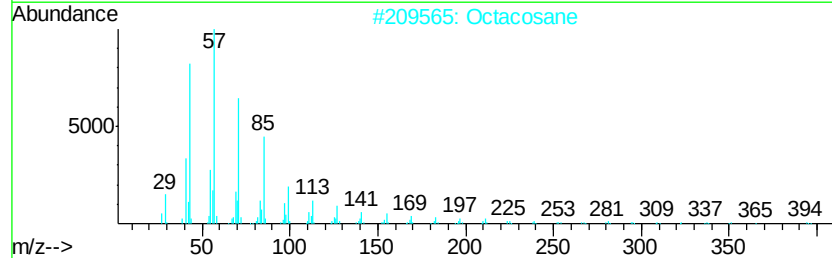
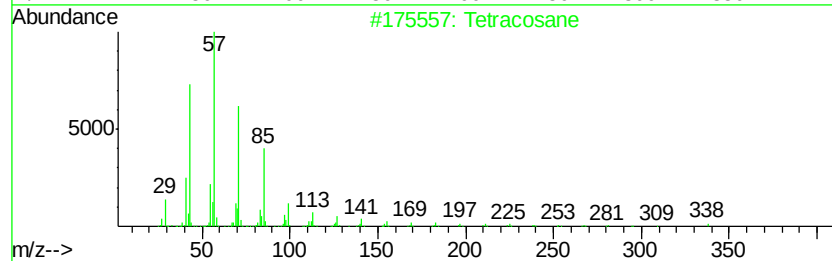
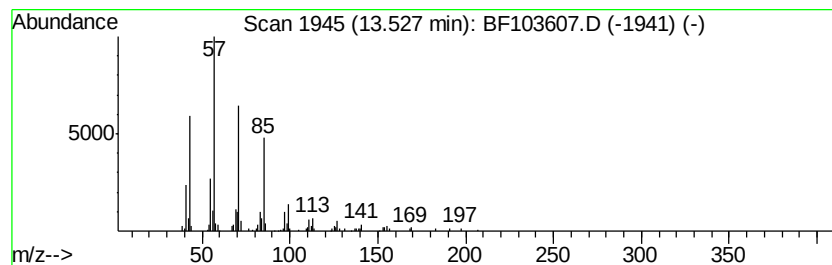
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.91 ng	138934	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Octacosane	394	C28H58	000630-02-4	90
3		Heneicosane	296	C21H44	000629-94-7	87
4		Tetratetracontane	619	C44H90	007098-22-8	83
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103607.D
Acq On : 13 Mar 2018 16:35
Operator : SJ/JU
Sample : J1753-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

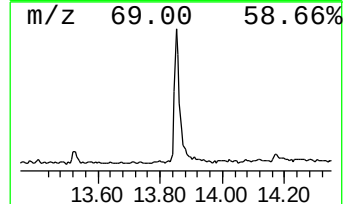
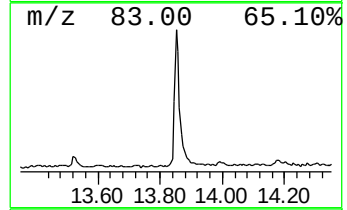
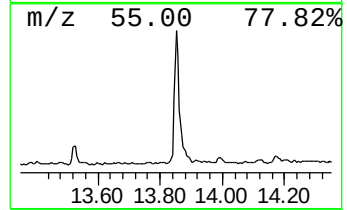
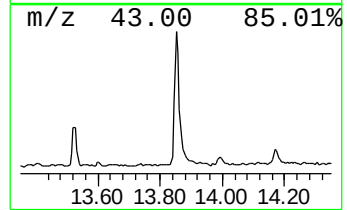
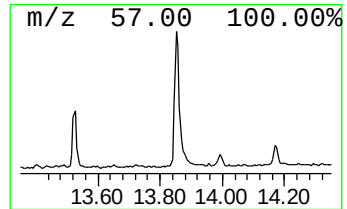
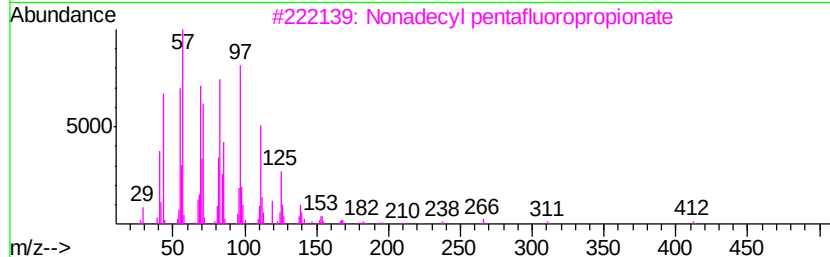
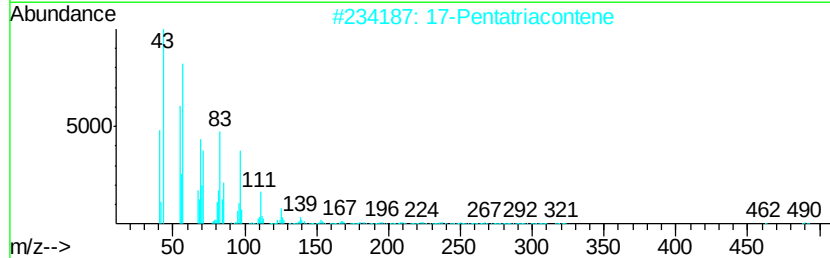
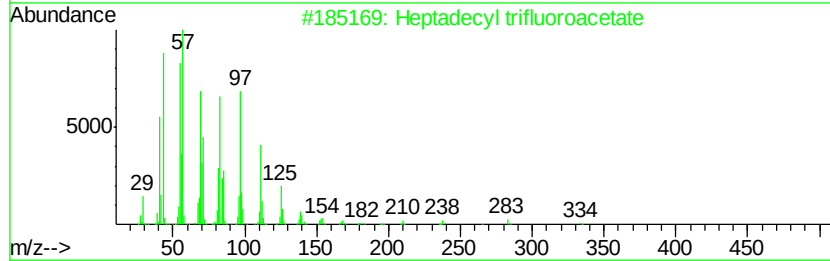
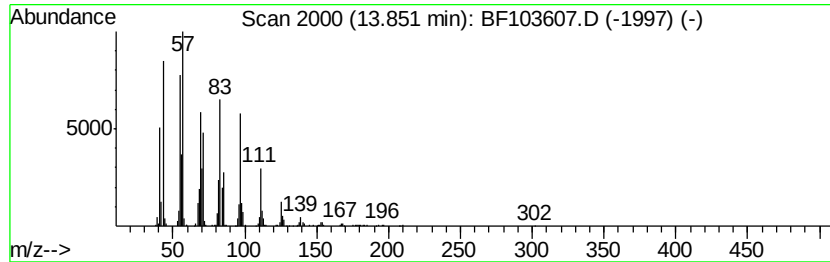
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	16.21 ng	774600	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031318\
Data File : BF103607.D
Acq On : 13 Mar 2018 16:35
Operator : SJ/JU
Sample : J1753-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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
unknown6.63	6.63	70.3	ng	2990870	1	6.86	851297	20.0
Propanoic acid, 2...	9.07	2.4	ng	150145	3	9.90	1235690	20.0
Vanillin	9.40	2.8	ng	171899	3	9.90	1235690	20.0
Phthalic acid, he...	11.54	2.9	ng	189513	4	11.40	1324760	20.0
Heptadecane	12.83	2.3	ng	110766	5	14.05	955664	20.0
Octacosane	13.18	5.1	ng	243835	5	14.05	955664	20.0
Tetracosane	13.53	2.9	ng	138934	5	14.05	955664	20.0
Heptadecyl triflu...	13.85	16.2	ng	774600	5	14.05	955664	20.0