

Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
 Data File : BF102989.D
 Acq On : 14 Feb 2018 15:09
 Operator : SJ/JU
 Sample : J1541-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-B-1-3

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-BF020318.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	2.169	8	14	29	rVB	823236	1160235	28.20%	3.176%
2	3.969	315	320	326	rVB	43739	54908	1.33%	0.150%
3	5.116	511	515	526	rVB	109141	143820	3.50%	0.394%
4	5.498	575	580	584	rBV	3848994	4114426	100.00%	11.263%
5	6.510	746	752	762	rBV	3603470	4103650	99.74%	11.233%
6	6.645	771	775	779	rBV	3789287	3987944	96.93%	10.916%
7	6.875	810	814	818	rBV	1202886	959987	23.33%	2.628%
8	7.033	837	841	844	rBV	3396268	2997142	72.84%	8.204%
9	7.439	905	910	913	rBV	2645839	2634006	64.02%	7.210%
10	8.157	1028	1032	1035	rBV	1414577	1290168	31.36%	3.532%
11	8.180	1035	1036	1042	rVB	299779	159983	3.89%	0.438%
12	8.869	1150	1153	1159	rBV	193034	160042	3.89%	0.438%
13	8.969	1166	1170	1174	rVB	77621	63852	1.55%	0.175%
14	9.233	1210	1215	1218	rBV	3794346	3397090	82.57%	9.299%
15	9.304	1224	1227	1229	rBV	60524	46637	1.13%	0.128%
16	9.333	1229	1232	1237	rVB	66872	63394	1.54%	0.174%
17	9.569	1264	1272	1275	rBV4	30184	51664	1.26%	0.141%
18	9.622	1278	1281	1284	rBV	392955	311724	7.58%	0.853%
19	9.833	1309	1317	1321	rBV	159097	147932	3.60%	0.405%
20	9.916	1327	1331	1334	rBV	1234459	1100101	26.74%	3.011%
21	9.945	1334	1336	1340	rVB	256819	187696	4.56%	0.514%
22	10.116	1362	1365	1369	rVB	181811	164885	4.01%	0.451%
23	10.333	1399	1402	1405	rVB	192076	143341	3.48%	0.392%
24	10.463	1420	1424	1429	rVB	308889	277683	6.75%	0.760%
25	10.551	1433	1439	1442	rBV2	57895	79435	1.93%	0.217%
26	10.704	1461	1465	1468	rBV	1802500	1619872	39.37%	4.434%
27	10.804	1480	1482	1491	rVB	147242	184552	4.49%	0.505%
28	10.957	1505	1508	1511	rVB	46443	44521	1.08%	0.122%
29	11.257	1555	1559	1561	rBV	86800	76394	1.86%	0.209%
30	11.286	1561	1564	1569	rVB3	40536	63577	1.55%	0.174%
31	11.404	1580	1584	1586	rBV	901684	903702	21.96%	2.474%
32	11.421	1586	1587	1592	rVV	562054	468957	11.40%	1.284%
33	11.474	1593	1596	1600	rVB	308453	264596	6.43%	0.724%
34	11.627	1616	1622	1628	rBV	140230	150213	3.65%	0.411%

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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-BF020318.M
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35	11.680	1628	1631	1639	rVV	47954	47497	1.15%	0.130%
36	11.927	1666	1673	1679	rBV6	34231	78035	1.90%	0.214%
37	12.015	1685	1688	1691	rBV	42964	42695	1.04%	0.117%
38	12.615	1786	1790	1793	rBV	238001	218413	5.31%	0.598%
39	12.845	1823	1829	1832	rBV	189279	201194	4.89%	0.551%
40	12.986	1848	1853	1856	rBV	2196609	2084198	50.66%	5.705%
41	13.862	1999	2002	2012	rBV	379256	421902	10.25%	1.155%
42	14.039	2028	2032	2035	rBV	927471	885498	21.52%	2.424%
43	14.062	2035	2036	2042	rVB	64434	52764	1.28%	0.144%
44	14.498	2107	2110	2115	rBV2	79153	84012	2.04%	0.230%
45	15.521	2279	2284	2294	rVB	558637	744140	18.09%	2.037%
46	16.015	2366	2368	2378	rVB5	52786	92884	2.26%	0.254%

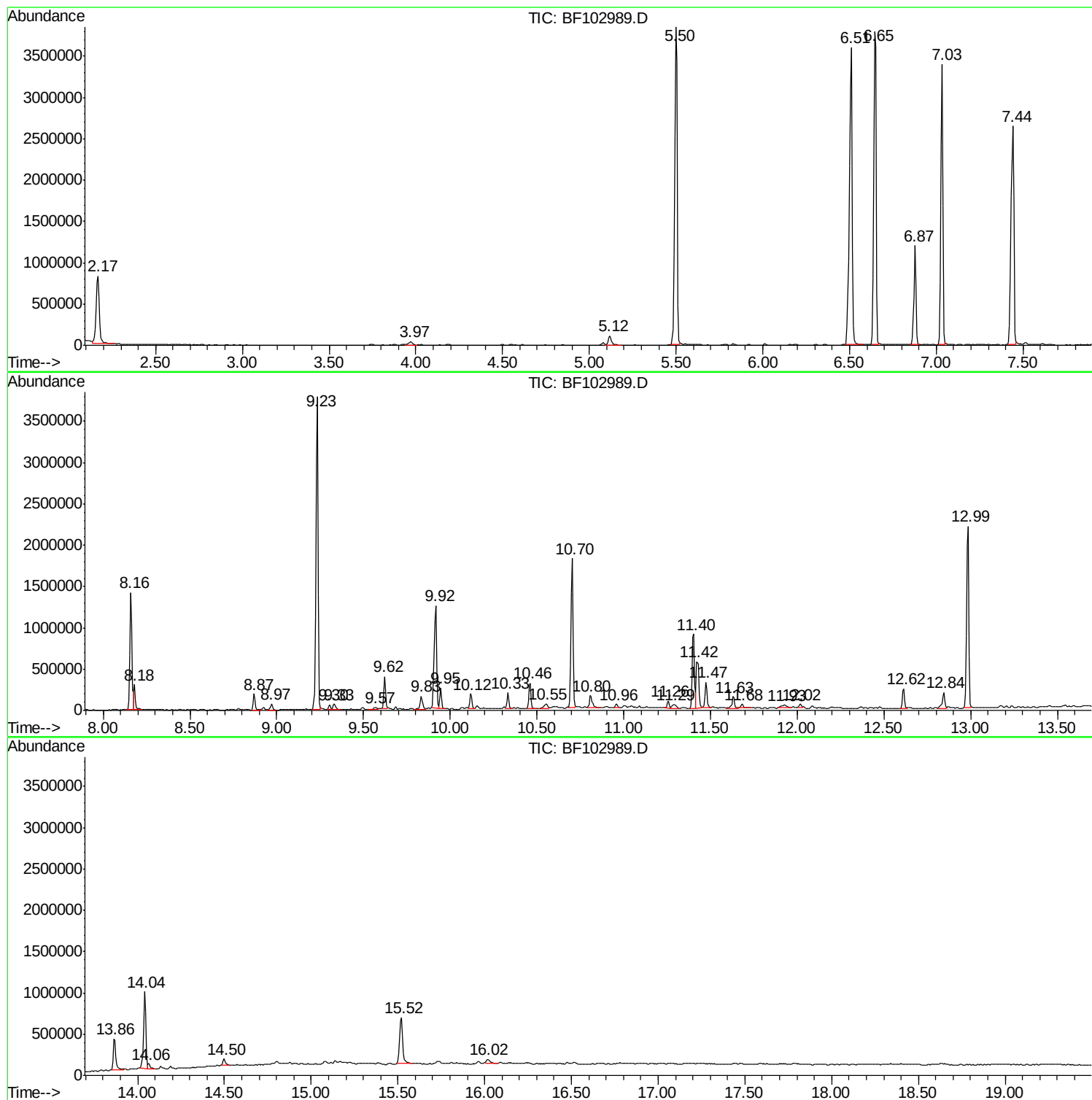
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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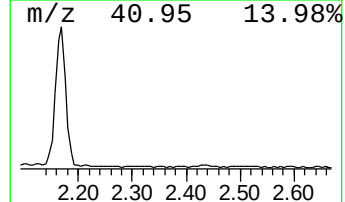
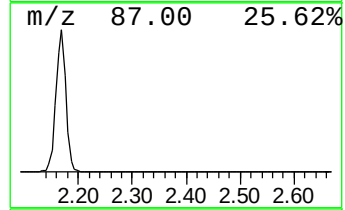
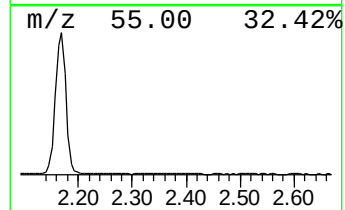
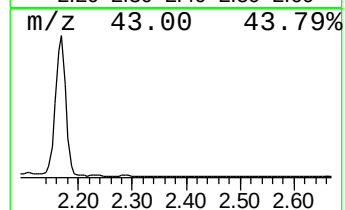
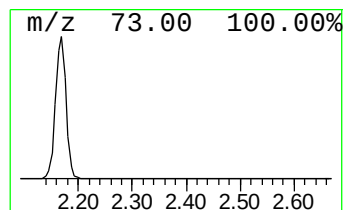
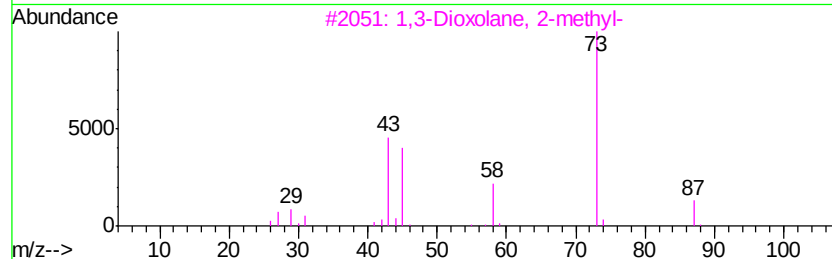
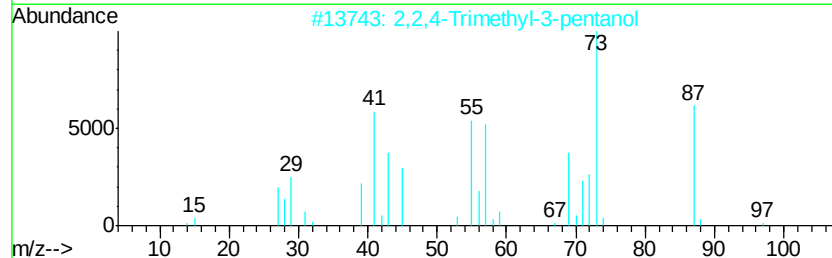
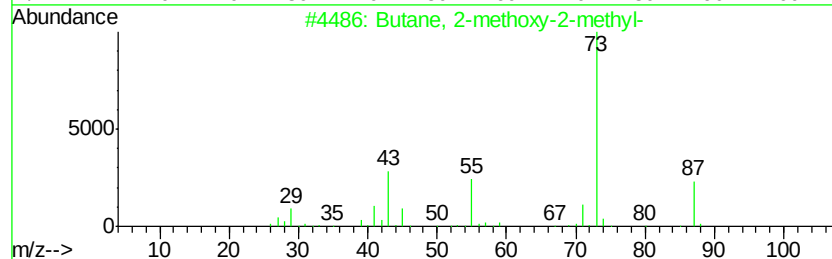
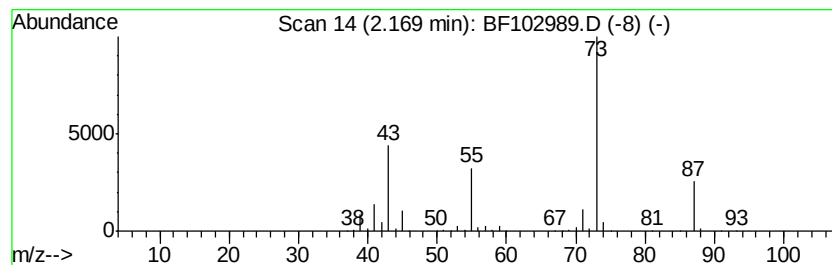
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	24.17 ng	1160240	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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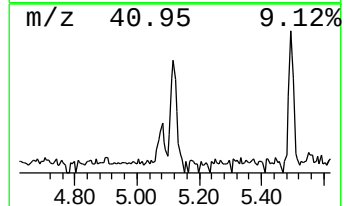
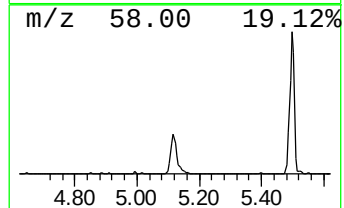
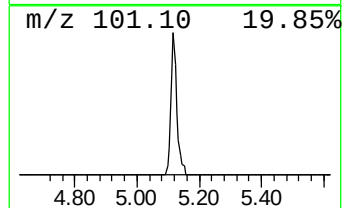
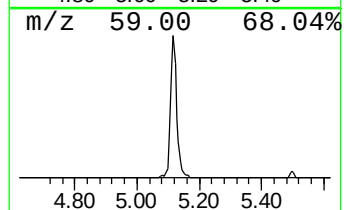
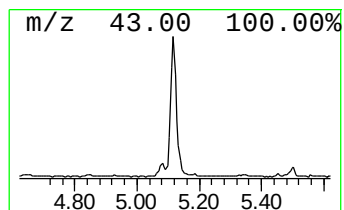
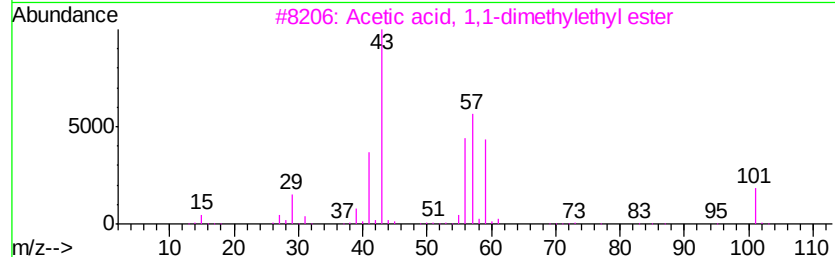
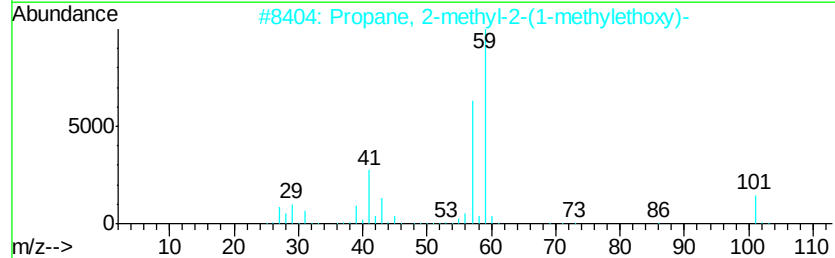
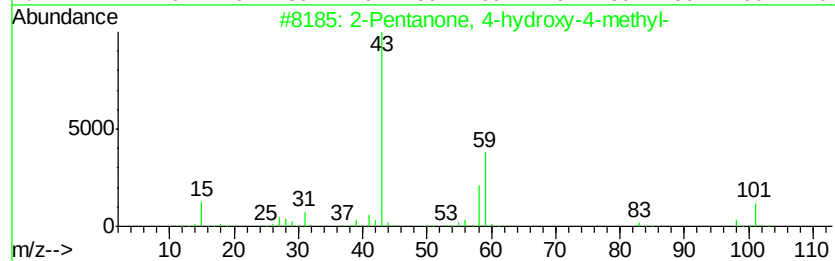
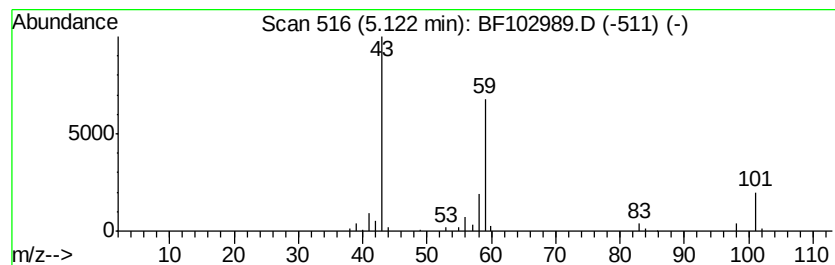
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.00 ng	143820	1,4-Dichlorobenzene-d4	6.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28



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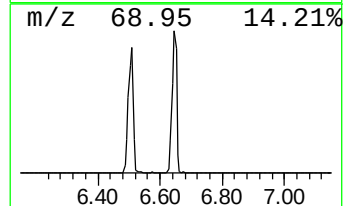
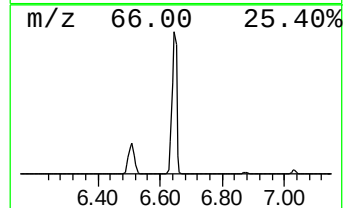
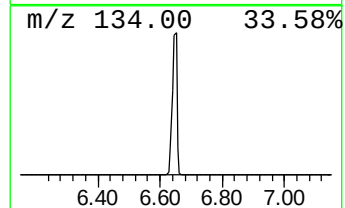
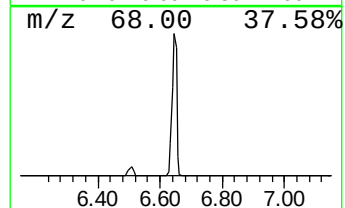
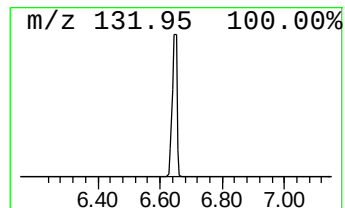
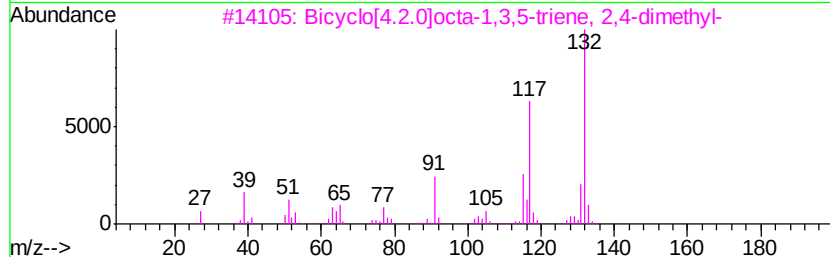
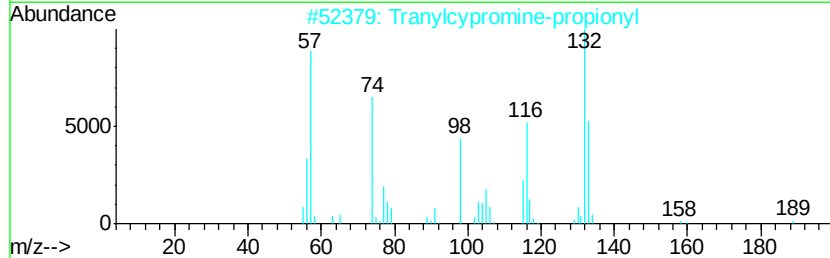
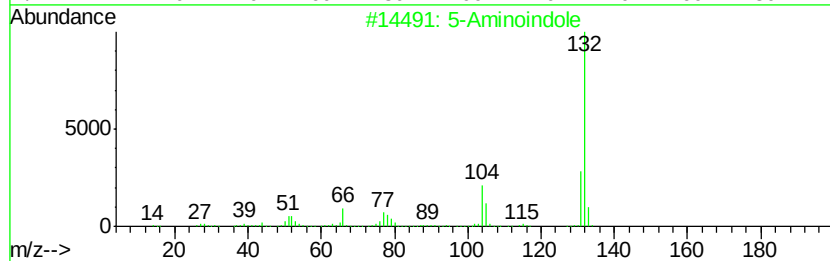
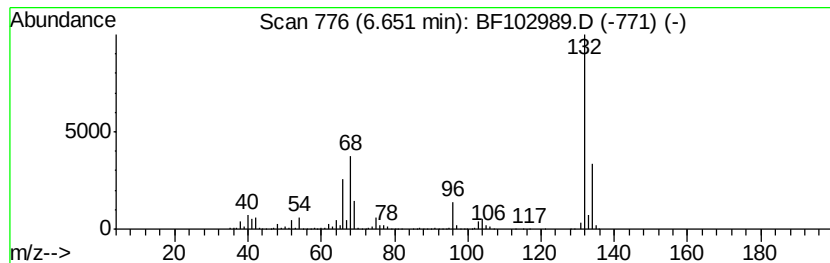
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	83.08 ng	3987940	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
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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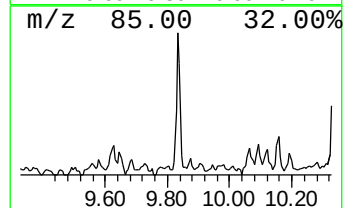
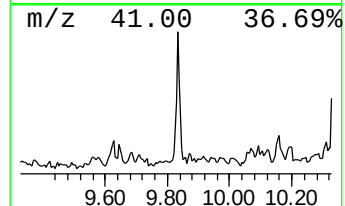
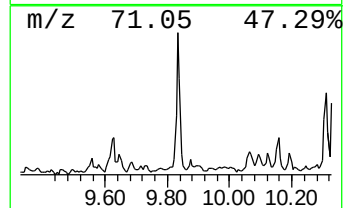
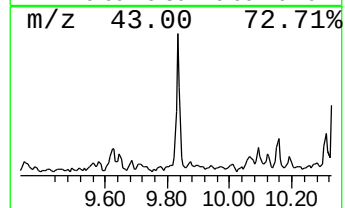
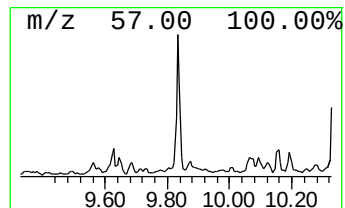
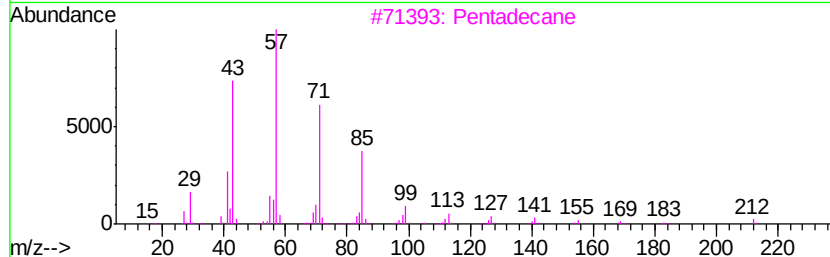
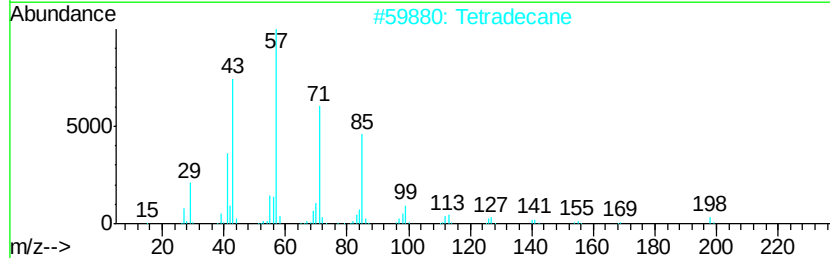
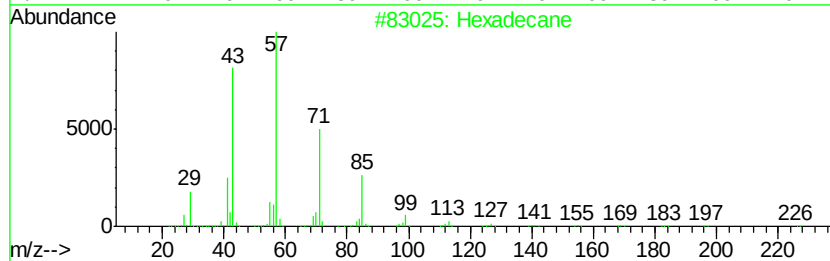
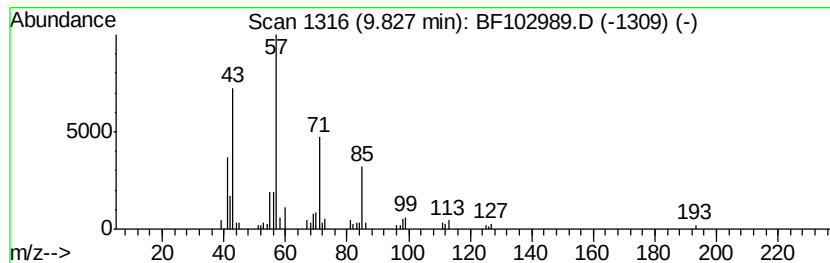
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.69 ng	147932	Acenaphthene-d10	9.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	87
2		Tetradecane	198	C14H30	000629-59-4	86
3		Pentadecane	212	C15H32	000629-62-9	80
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5		Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64



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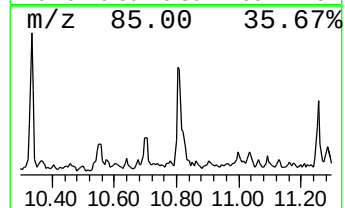
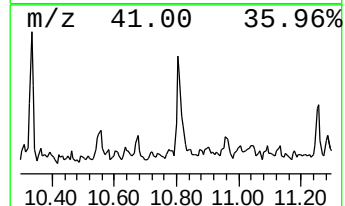
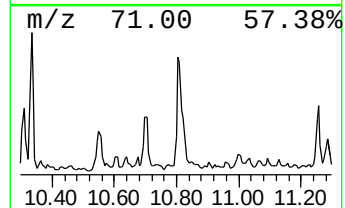
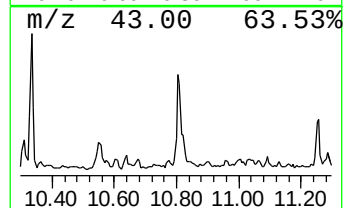
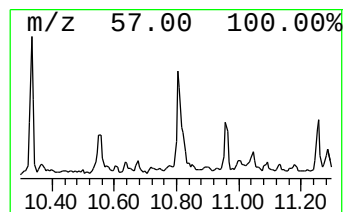
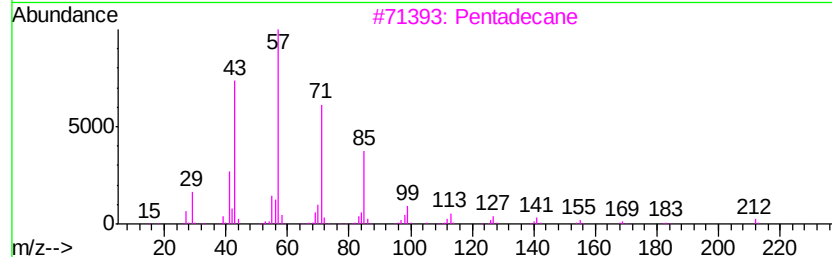
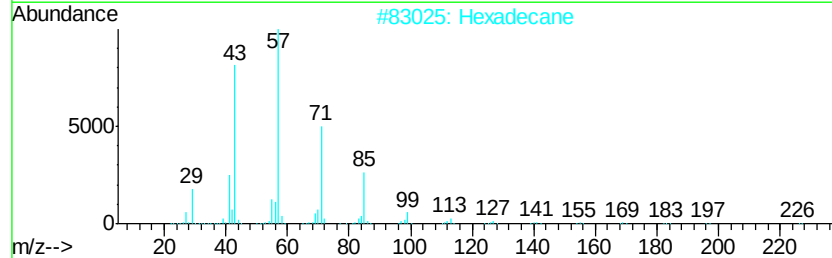
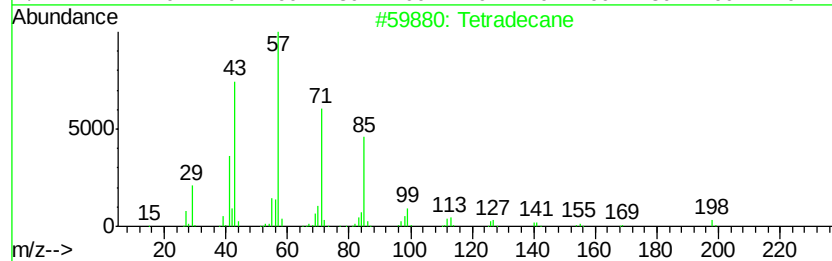
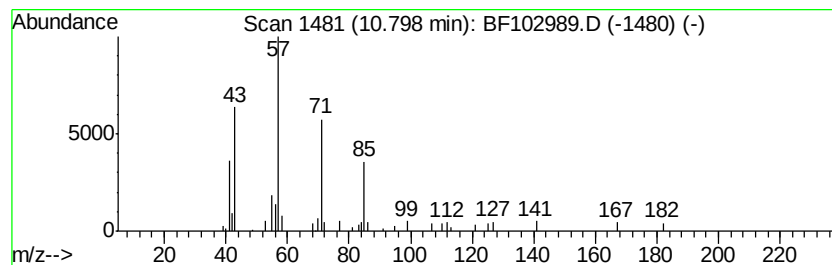
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.80	4.08 ng	184552	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021418\
Data File : BF102989.D
Acq On : 14 Feb 2018 15:09
Operator : SJ/JU
Sample : J1541-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

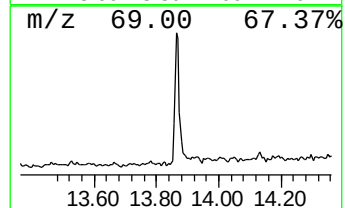
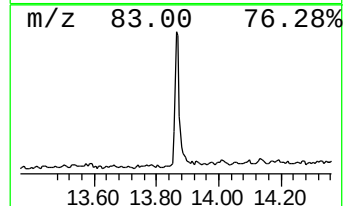
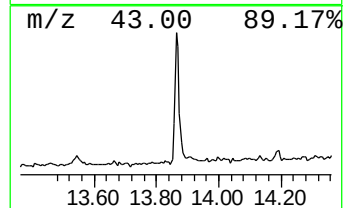
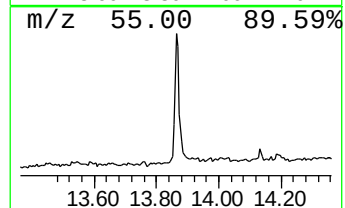
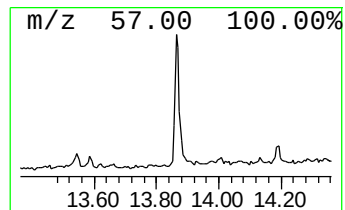
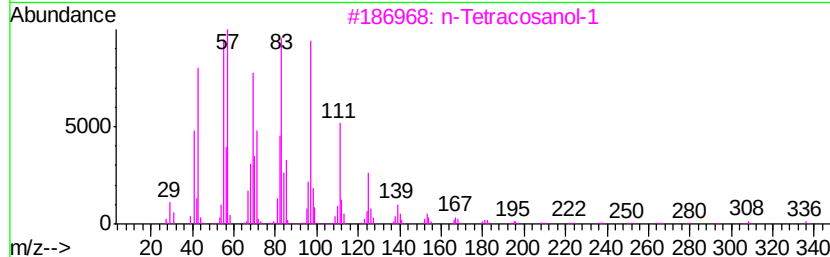
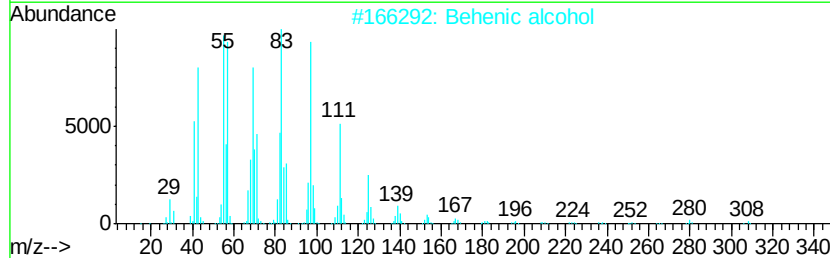
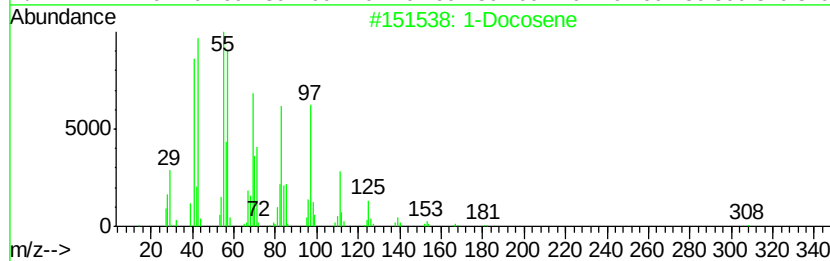
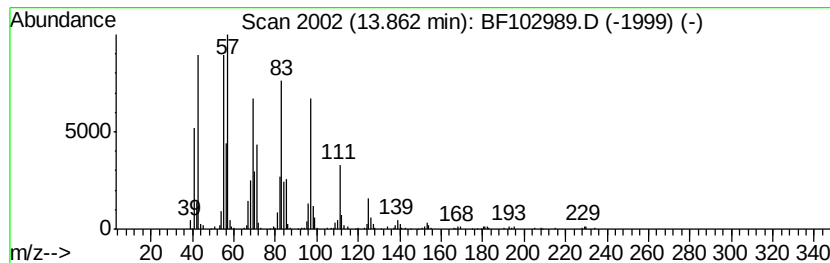
Instrument :
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ClientSampleId :
SAMPLE-B-1-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	9.53 ng	421902	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	Octacosanol	410	C28H58O	000557-61-9	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF021418\
Data File : BF102989.D
Acq On : 14 Feb 2018 15:09
Operator : SJ/JU
Sample : J1541-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

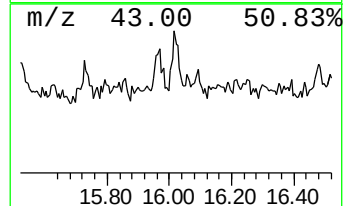
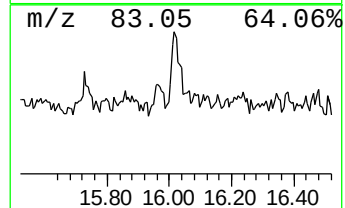
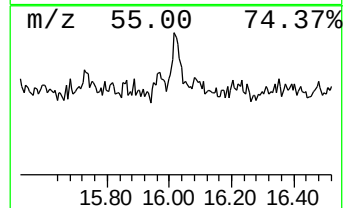
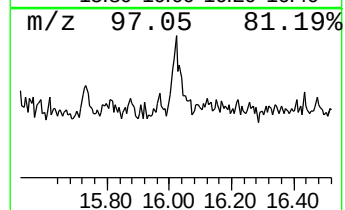
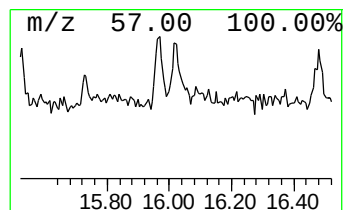
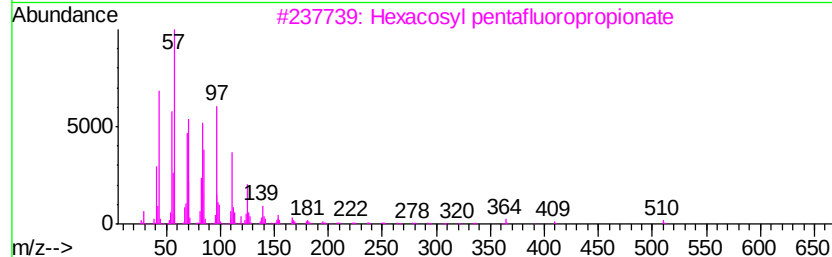
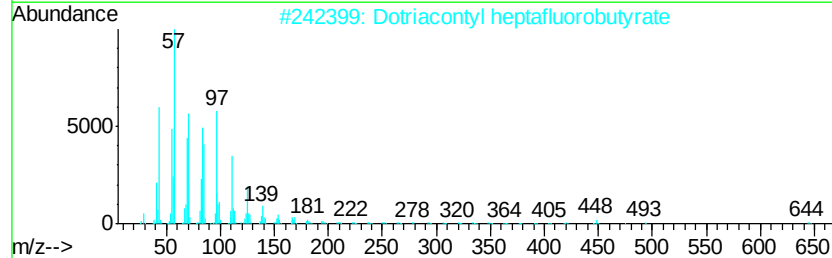
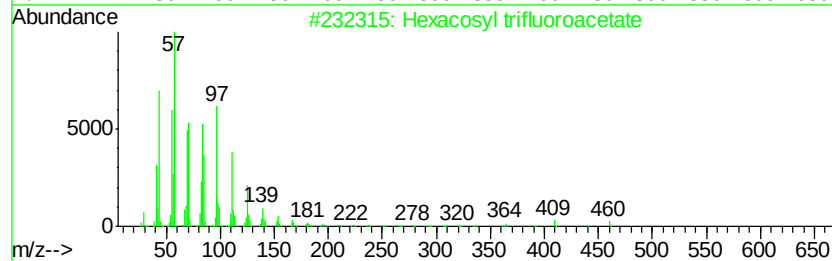
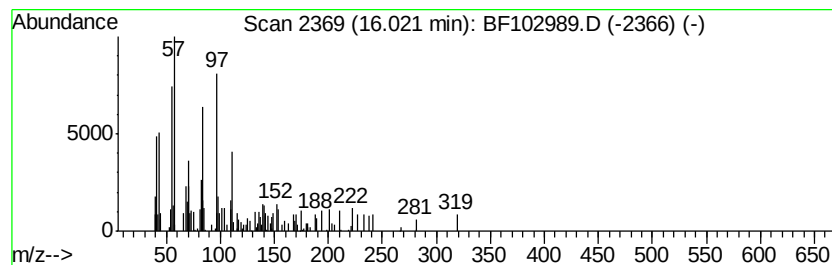
Instrument :
BNA_F
ClientSampleId :
SAMPLE-B-1-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.02	2.50 ng	92884	Perylene-d12	15.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	52
2	Dotriacontyl heptafluorobutyrte	662	C36H65F7O2	1000351-84-2	49
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	49
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	49
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021418\
Data File : BF102989.D
Acq On : 14 Feb 2018 15:09
Operator : SJ/JU
Sample : J1541-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-B-1-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.17	24.2	ng	1160240	1	6.87	959987	20.0
2-Pentanone, 4-hy...	5.12	3.0	ng	143820	1	6.87	959987	20.0
unknown6.65	6.65	83.1	ng	3987940	1	6.87	959987	20.0
Hexadecane	9.83	2.7	ng	147932	3	9.92	1100100	20.0
Tetradecane	10.80	4.1	ng	184552	4	11.40	903702	20.0
1-Docosene	13.86	9.5	ng	421902	5	14.04	885498	20.0
Hexacosyl trifluo...	16.02	2.5	ng	92884	6	15.52	744140	20.0