

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
 Data File : BF096793.D
 Acq On : 15 Jul 2017 1:19
 Operator : SJ/JU
 Sample : I4187-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CI-SB3-0-2

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-BF071317.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	4.804	475	479	491	rVB	203364	280314	11.10%	1.351%
2	5.240	548	553	556	rBV	2332412	2524645	100.00%	12.170%
3	6.275	724	729	732	rBV	2168642	2130688	84.40%	10.271%
4	6.398	745	750	753	rBV	2298676	2151390	85.22%	10.371%
5	6.622	785	788	792	rBV	676595	564293	22.35%	2.720%
6	6.781	811	815	818	rBV	1891918	1654154	65.52%	7.974%
7	7.187	879	884	887	rBV	1463542	1365605	54.09%	6.583%
8	7.904	1002	1006	1010	rBV	1079447	885553	35.08%	4.269%
9	8.987	1185	1190	1193	rBV	2443755	2364056	93.64%	11.396%
10	9.375	1253	1256	1259	rBV	200566	153023	6.06%	0.738%
11	9.651	1299	1303	1307	rBV	874081	825597	32.70%	3.980%
12	10.104	1377	1380	1383	rVB	34779	26469	1.05%	0.128%
13	10.439	1433	1437	1440	rBV	1148690	1013894	40.16%	4.888%
14	10.575	1457	1460	1469	rBV	46037	47824	1.89%	0.231%
15	11.128	1551	1554	1557	rBV	666612	616905	24.44%	2.974%
16	11.151	1557	1558	1561	rVB	44563	27975	1.11%	0.135%
17	11.675	1642	1647	1651	rBV2	65822	78165	3.10%	0.377%
18	12.333	1757	1759	1764	rVB	61866	58956	2.34%	0.284%
19	12.563	1790	1798	1802	rBV	72640	84067	3.33%	0.405%
20	12.716	1820	1824	1827	rBV	1452204	1297132	51.38%	6.253%
21	13.622	1973	1978	1985	rBV2	173111	219621	8.70%	1.059%
22	13.757	1995	2001	2004	rBV2	756771	746987	29.59%	3.601%
23	13.863	2017	2019	2025	rBV6	15487	29111	1.15%	0.140%
24	13.951	2032	2034	2038	rVB5	20220	26050	1.03%	0.126%
25	14.180	2070	2073	2076	rBV5	15964	31379	1.24%	0.151%
26	14.257	2083	2086	2095	rVB	90444	115125	4.56%	0.555%
27	14.610	2140	2146	2148	rBV3	38954	54589	2.16%	0.263%
28	14.674	2154	2157	2160	rVB2	52601	45567	1.80%	0.220%
29	14.751	2168	2170	2174	rBV	29906	38714	1.53%	0.187%
30	14.868	2185	2190	2196	rVB2	114392	209368	8.29%	1.009%
31	15.027	2215	2217	2219	rVB	35631	28430	1.13%	0.137%
32	15.139	2231	2236	2241	rBV	542845	652793	25.86%	3.147%
33	15.463	2288	2291	2294	rBV5	21498	30551	1.21%	0.147%
34	15.580	2308	2311	2315	rVB	57721	73795	2.92%	0.356%

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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

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35	15.627	2315	2319	2325	rBV2	50265	103423	4.10%	0.499%
36	16.039	2384	2389	2390	rBV5	20050	31997	1.27%	0.154%
37	16.433	2452	2456	2459	rBV4	20814	35480	1.41%	0.171%
38	16.545	2471	2475	2479	rBV4	21541	38271	1.52%	0.184%
39	16.704	2495	2502	2503	rBV7	20647	46865	1.86%	0.226%
40	17.821	2685	2692	2694	rBV7	15136	35518	1.41%	0.171%

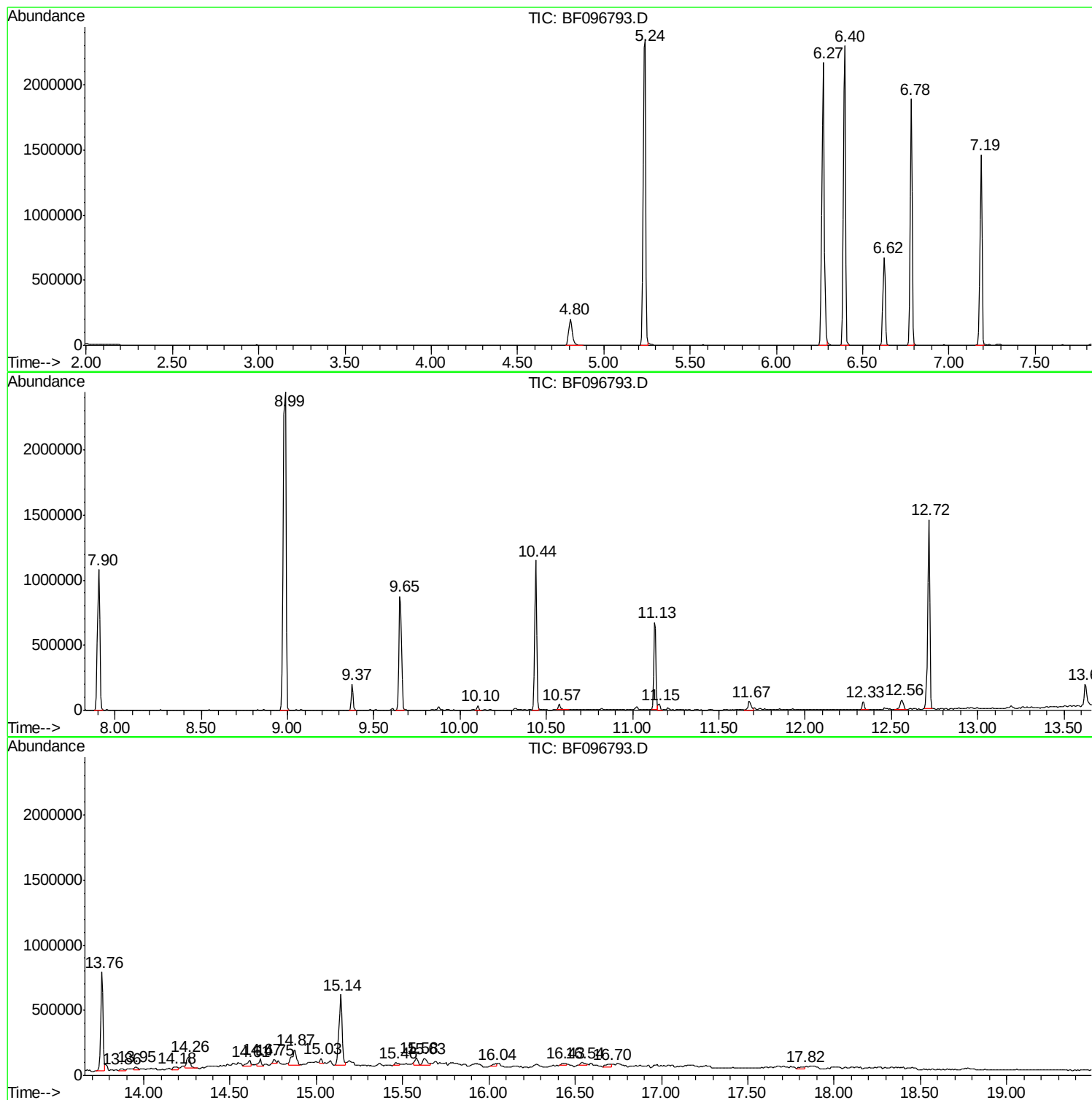
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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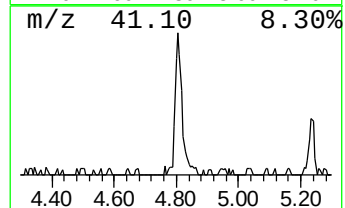
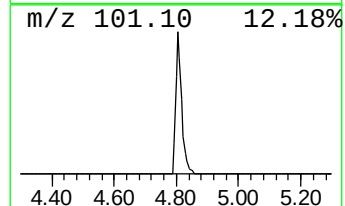
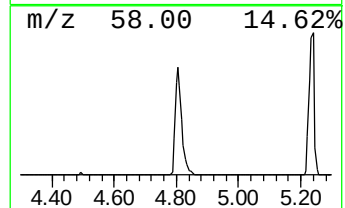
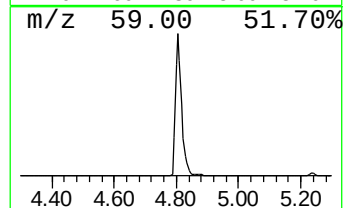
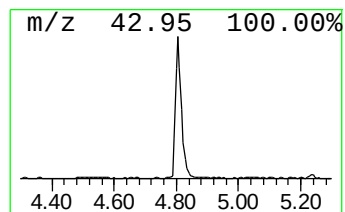
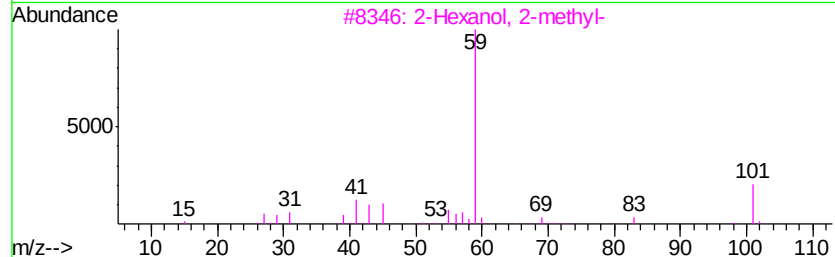
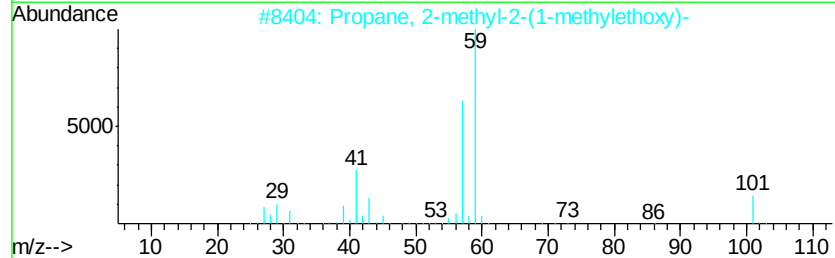
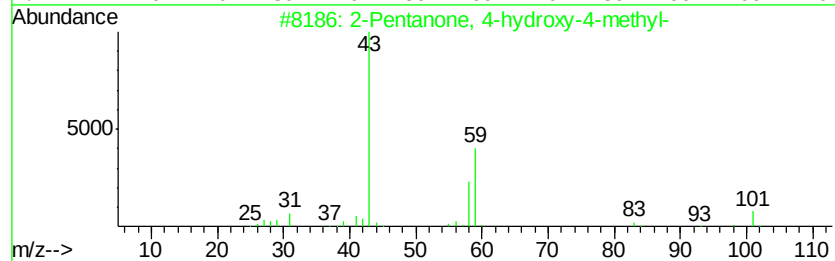
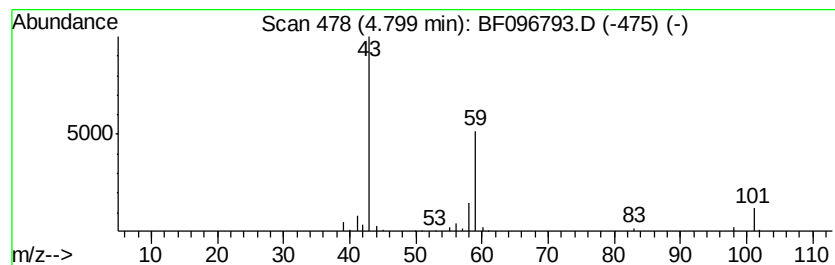
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.80	9.94 ng	280314	1,4-Dichlorobenzene-d4	6.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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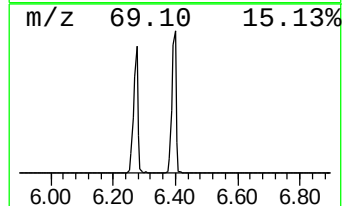
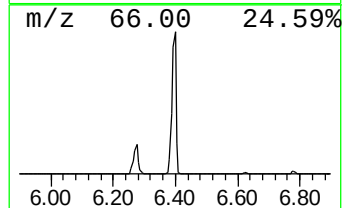
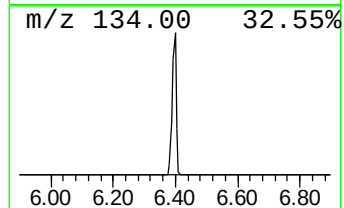
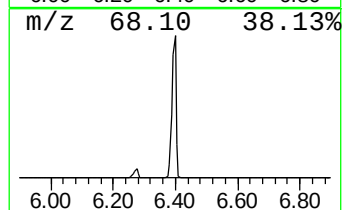
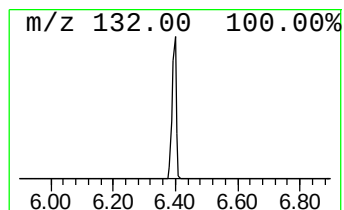
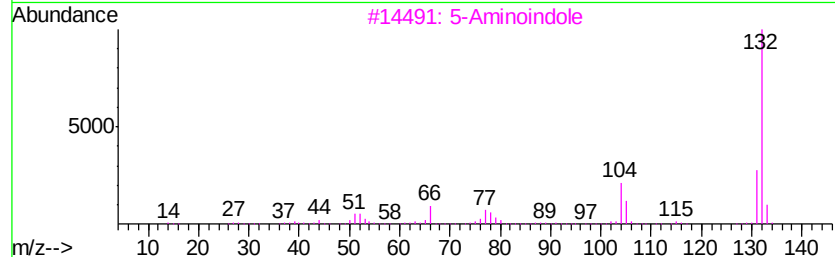
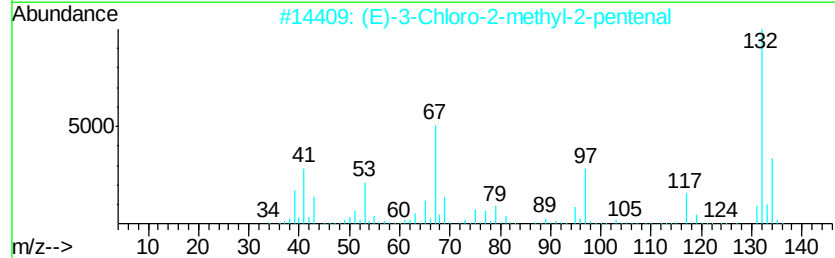
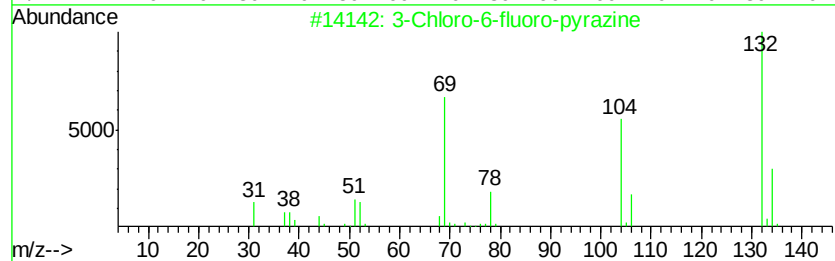
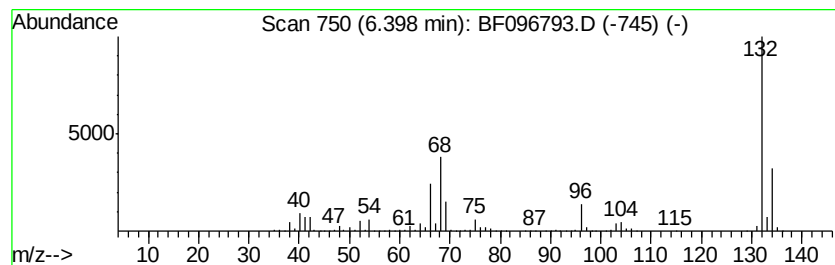
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	76.25 ng	2151390	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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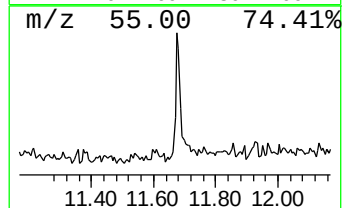
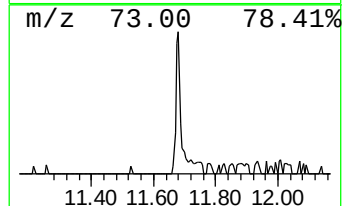
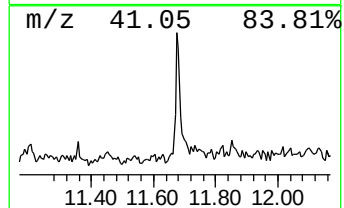
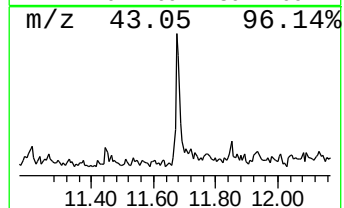
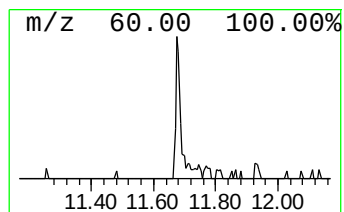
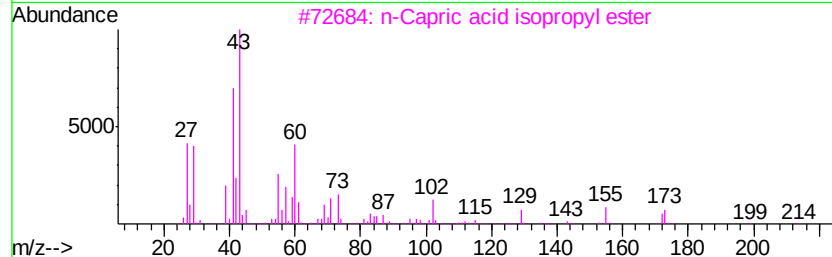
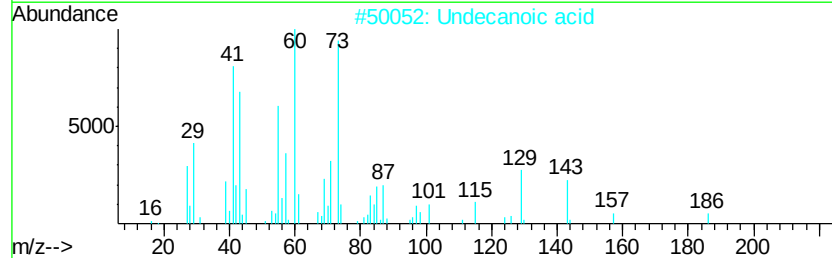
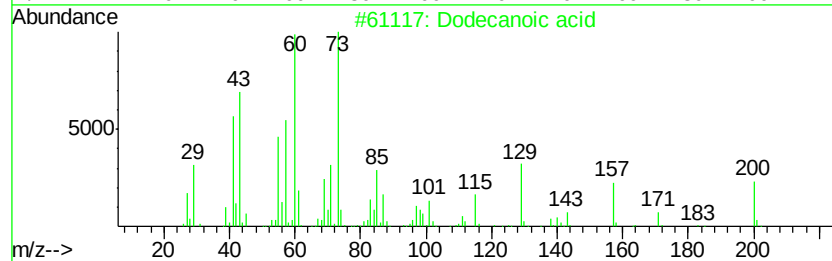
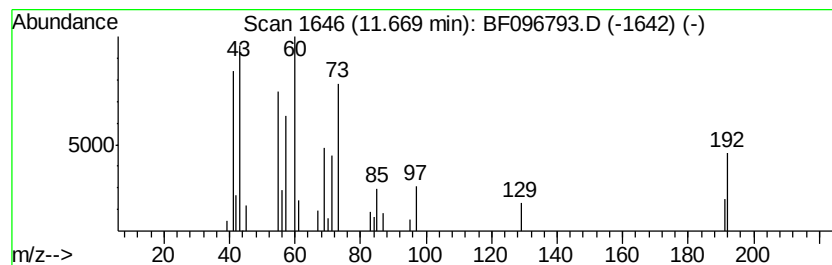
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.53 ng	78165	Phenanthrene-d10	11.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	72
2		Undecanoic acid	186	C11H22O2	000112-37-8	64
3		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	59
4		n-Decanoic acid	172	C10H20O2	000334-48-5	59
5		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	53



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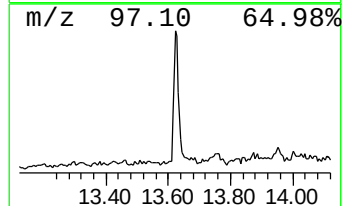
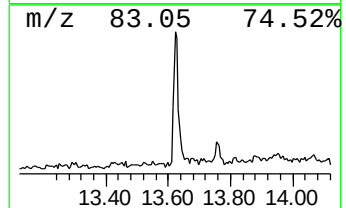
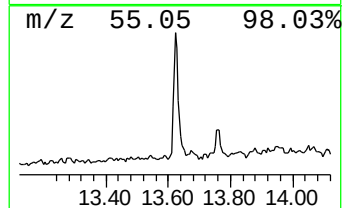
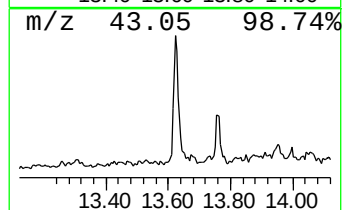
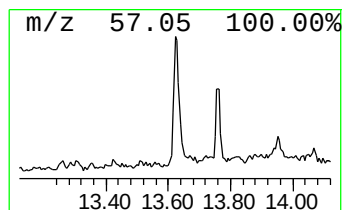
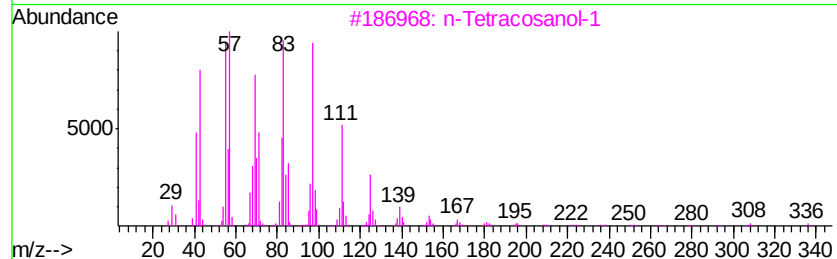
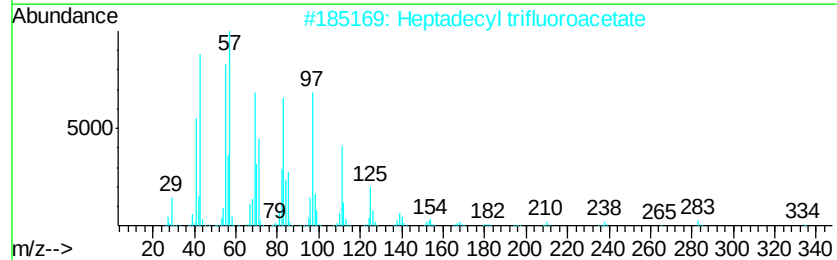
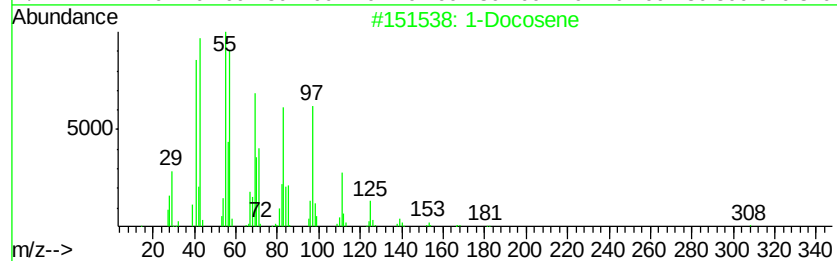
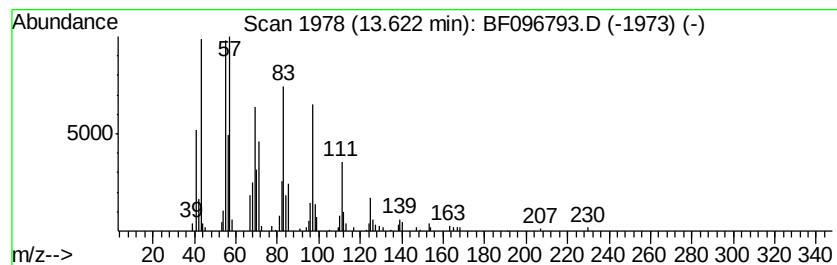
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.62	5.88 ng	219621	Chrysene-d12	13.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Octacosanol	410	C28H58O	000557-61-9	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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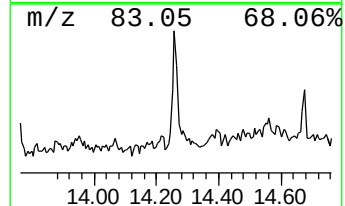
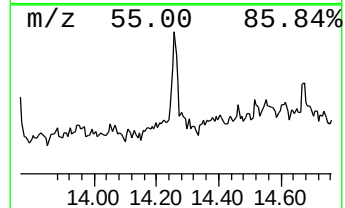
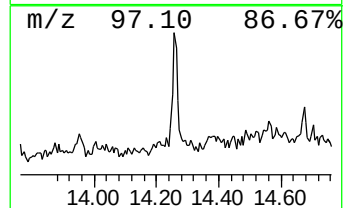
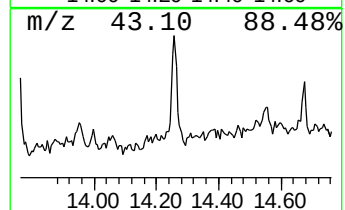
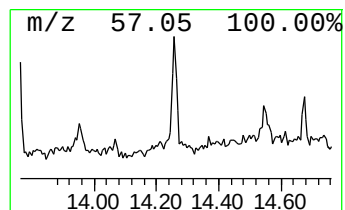
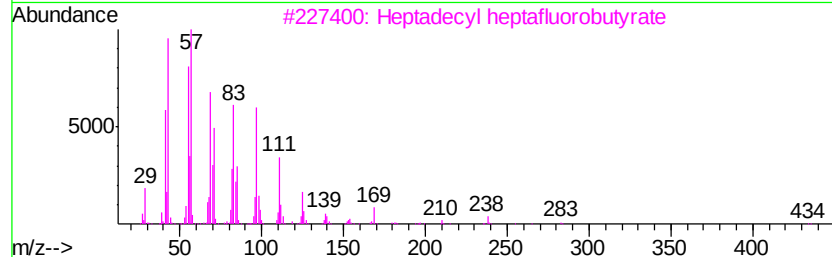
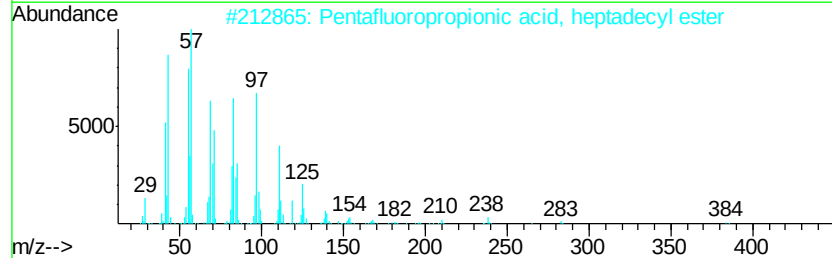
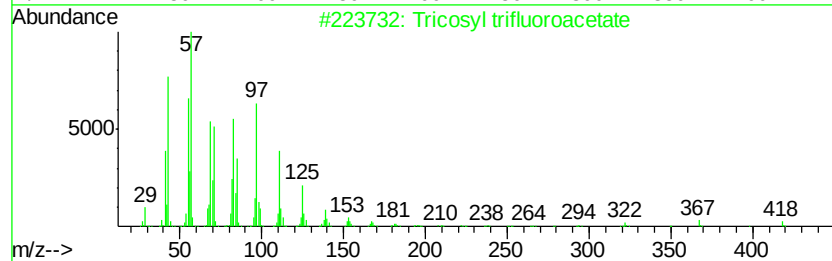
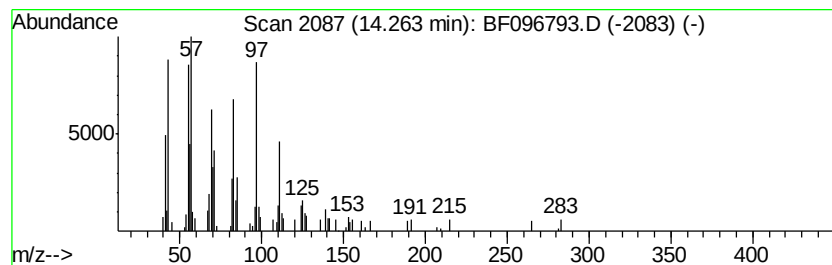
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tricosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.08 ng	115125	Chrysene-d12	13.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	93
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096793.D
Acq On : 15 Jul 2017 1:19
Operator : SJ/JU
Sample : I4187-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB3-0-2

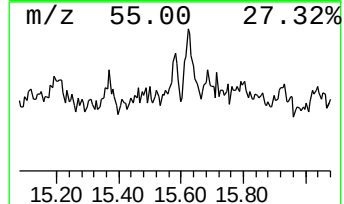
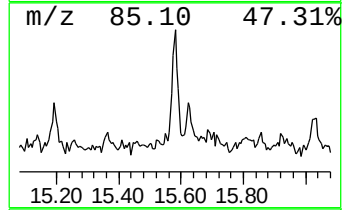
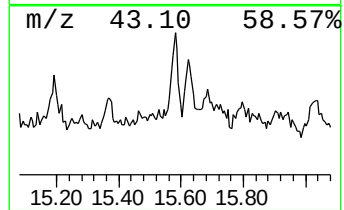
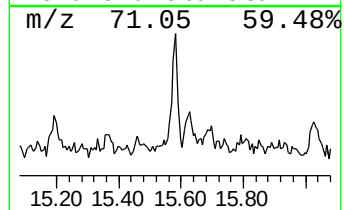
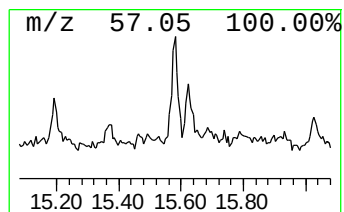
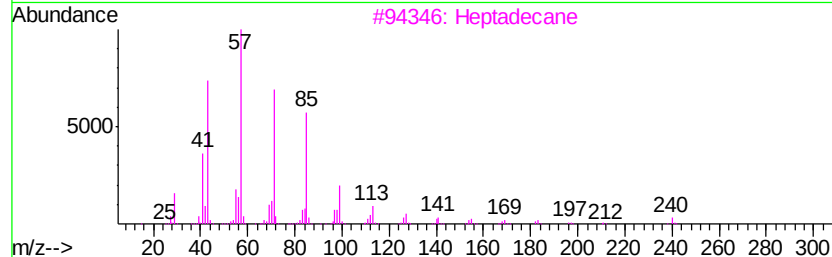
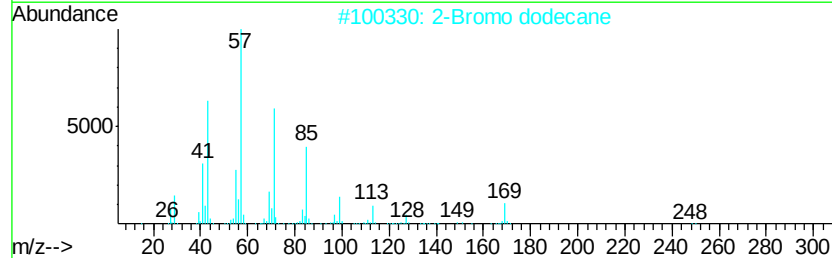
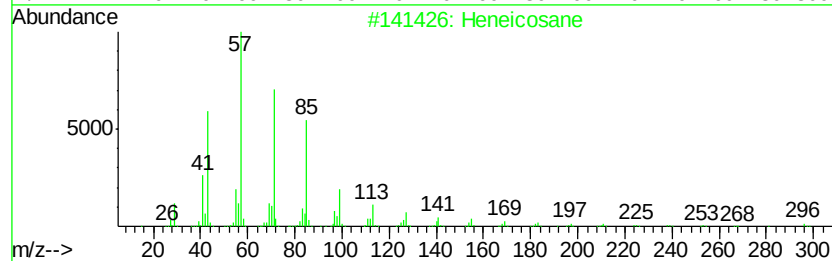
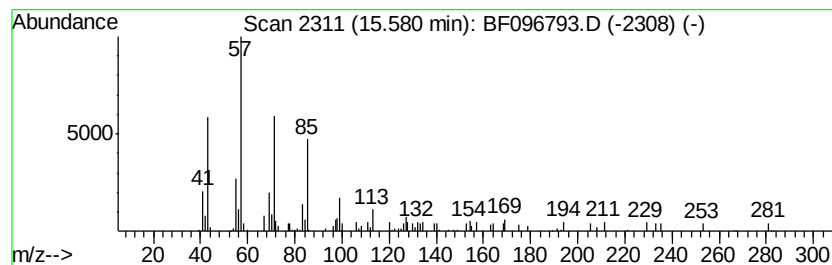
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.26 ng	73795	Perylene-d12	15.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	74
2	2-Bromo dodecane		248	C12H25Br	013187-99-0	72
3	Heptadecane		240	C17H36	000629-78-7	72
4	Pentacosane		352	C25H52	000629-99-2	72
5	Tetratetracontane		619	C44H90	007098-22-8	72



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096793.D
Acq On : 15 Jul 2017 1:19
Operator : SJ/JU
Sample : I4187-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

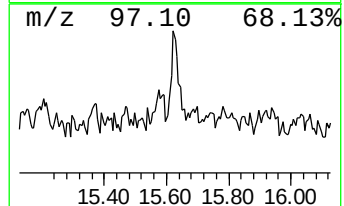
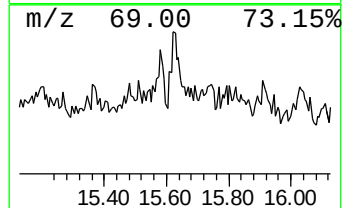
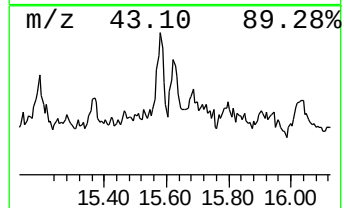
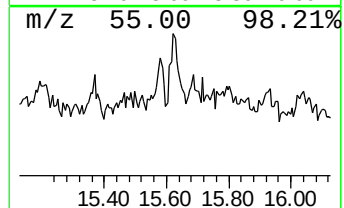
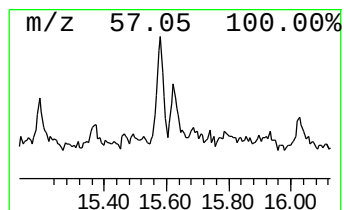
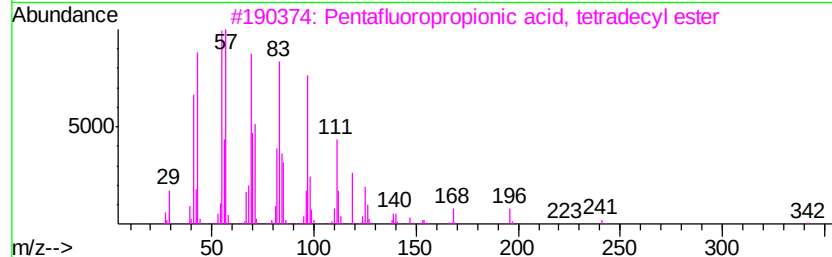
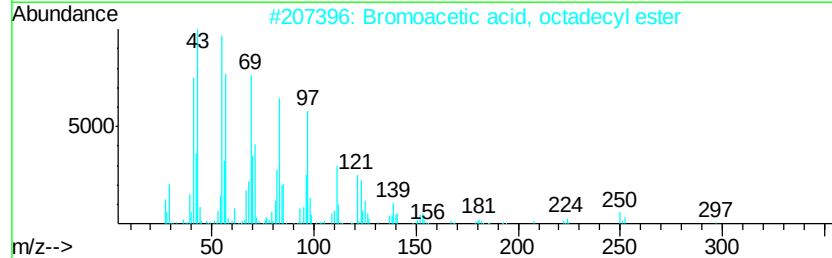
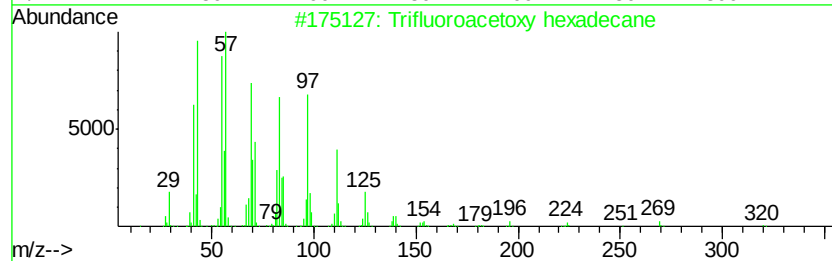
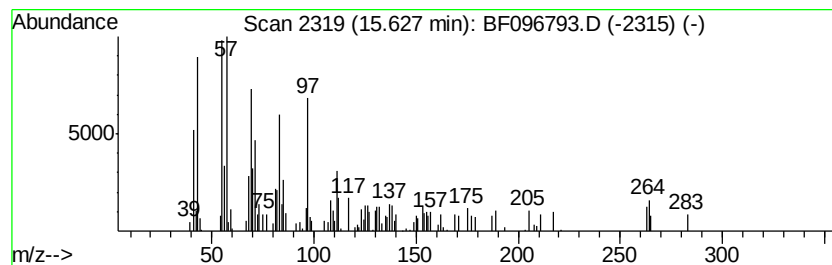
Instrument :
BNA_F
ClientSampleId :
CI-SB3-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.63	3.17 ng	103423	Perylene-d12	15.14		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	83
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	80
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	80



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
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Acq On : 15 Jul 2017 1:19
Operator : SJ/JU
Sample : I4187-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB3-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
2-Pentanone, 4-hy...	4.80	9.9	ng	280314	1	6.62	564293	20.0
unknown6.40	6.40	76.3	ng	2151390	1	6.62	564293	20.0
Dodecanoic acid	11.67	2.5	ng	78165	4	11.13	616905	20.0
1-Docosene	13.62	5.9	ng	219621	5	13.76	746987	20.0
Tricosyl trifluor...	14.26	3.1	ng	115125	5	13.76	746987	20.0
Heneicosane	15.58	2.3	ng	73795	6	15.14	652793	20.0
Trifluoroacetoxy ...	15.63	3.2	ng	103423	6	15.14	652793	20.0