

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
 Data File : BF098924.D
 Acq On : 28 Sep 2017 23:24
 Operator : SJ/JU
 Sample : I5488-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-D

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-BF092317.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	2.251	24	28	43	rVB	183241	272009	7.43%	0.861%
2	4.045	327	333	337	rBV	216377	266768	7.29%	0.844%
3	5.151	517	521	533	rVB	722480	983170	26.86%	3.112%
4	5.545	582	588	591	rBV	3428031	3591792	98.12%	11.370%
5	6.545	752	758	761	rBV	3090610	3660563	100.00%	11.588%
6	6.686	777	782	785	rBV	3465306	3602534	98.41%	11.404%
7	6.739	788	791	795	rBV	108182	86281	2.36%	0.273%
8	6.916	817	821	825	rVB	1203213	928428	25.36%	2.939%
9	7.075	843	848	851	rBV	2917936	2592802	70.83%	8.208%
10	7.310	885	888	892	rBV	109796	98435	2.69%	0.312%
11	7.481	906	917	920	rBV	2180034	2172156	59.34%	6.876%
12	7.575	931	933	936	rVB	56415	40368	1.10%	0.128%
13	8.198	1035	1039	1042	rBV	1419770	1176623	32.14%	3.725%
14	9.275	1216	1222	1225	rBV	3363716	3155177	86.19%	9.988%
15	9.663	1284	1288	1291	rBV	747528	612772	16.74%	1.940%
16	9.869	1317	1323	1326	rBV3	31064	50510	1.38%	0.160%
17	9.951	1333	1337	1341	rVB	1163411	1050610	28.70%	3.326%
18	10.374	1402	1409	1411	rBV	66977	71977	1.97%	0.228%
19	10.463	1421	1424	1427	rBV	102055	78732	2.15%	0.249%
20	10.592	1442	1446	1449	rBV	67036	70032	1.91%	0.222%
21	10.739	1468	1471	1475	rBV	1627964	1572056	42.95%	4.976%
22	10.857	1486	1491	1495	rBV3	127320	195458	5.34%	0.619%
23	11.292	1562	1565	1567	rBV	49962	42417	1.16%	0.134%
24	11.321	1567	1570	1577	rVB	67731	73138	2.00%	0.232%
25	11.439	1586	1590	1593	rBV	1004637	850875	23.24%	2.694%
26	11.463	1593	1594	1598	rVB	62886	37693	1.03%	0.119%
27	11.951	1673	1677	1686	rBV3	83242	104806	2.86%	0.332%
28	12.651	1793	1796	1800	rVB	95919	75738	2.07%	0.240%
29	12.880	1833	1835	1838	rBV	73954	57842	1.58%	0.183%
30	13.021	1855	1859	1863	rVB	2068312	1857583	50.75%	5.880%
31	13.904	2006	2009	2016	rVB	159142	171239	4.68%	0.542%
32	14.045	2031	2033	2035	rBV	66683	59026	1.61%	0.187%
33	14.080	2035	2039	2042	rVV	835099	754802	20.62%	2.389%
34	15.133	2214	2218	2221	rBV	41254	68352	1.87%	0.216%

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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	15.192	2225	2228	2231	rBV2	47498	48824	1.33%	0.155%
36	15.504	2278	2281	2287	rVB2	36472	51357	1.40%	0.163%
37	15.574	2288	2293	2304	rVB	638568	829177	22.65%	2.625%
38	16.027	2367	2370	2376	rVB2	57931	82823	2.26%	0.262%
39	16.551	2455	2459	2465	rVB3	54017	94755	2.59%	0.300%

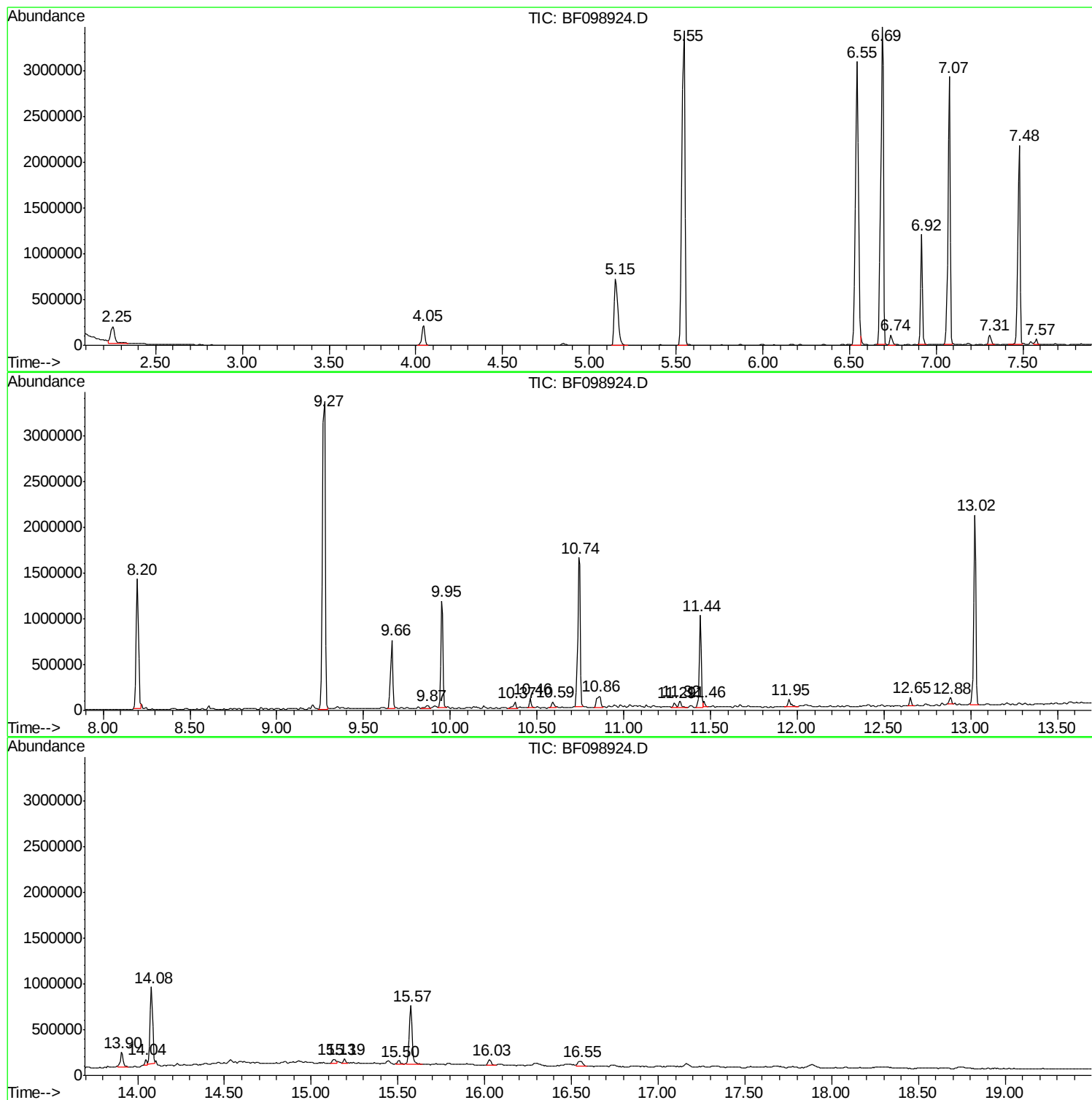
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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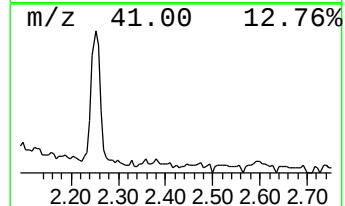
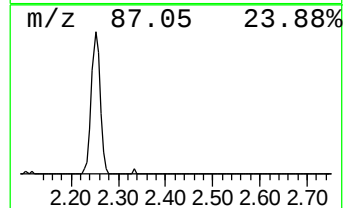
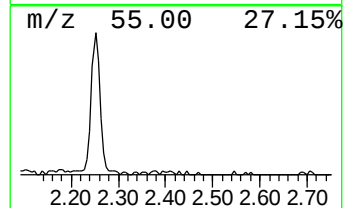
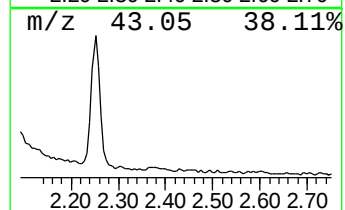
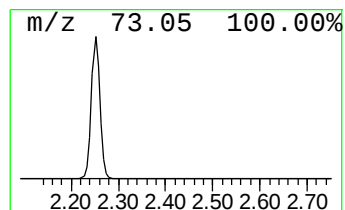
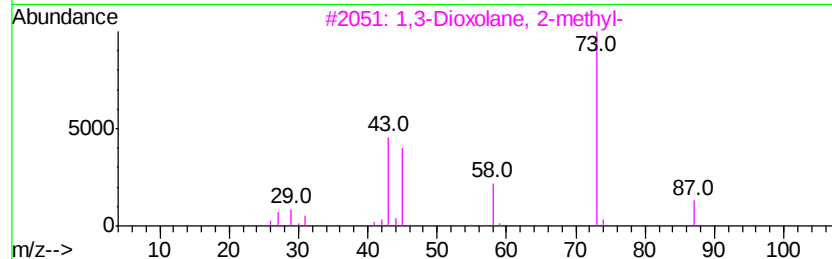
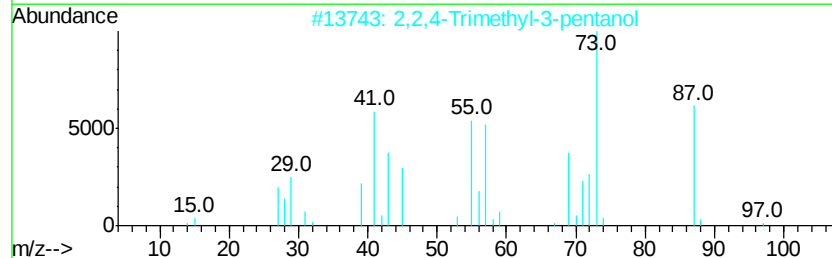
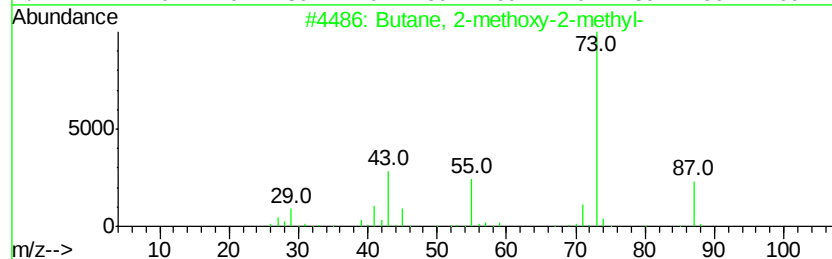
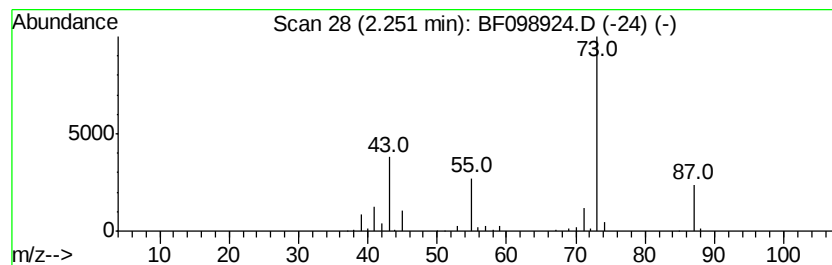
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	5.86 ng	272009	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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	25
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12



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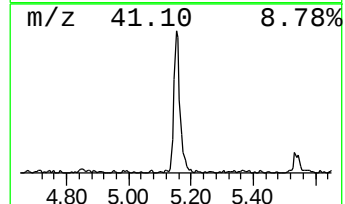
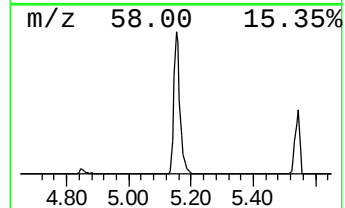
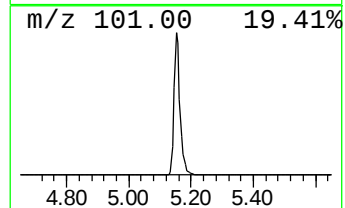
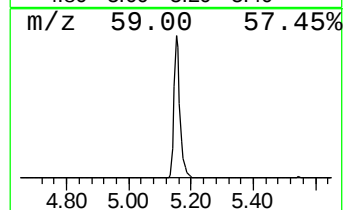
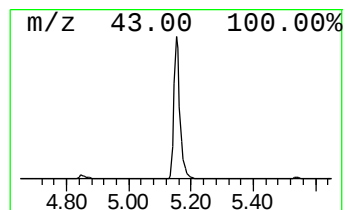
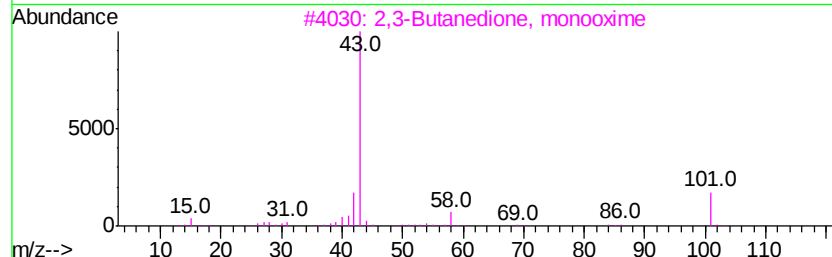
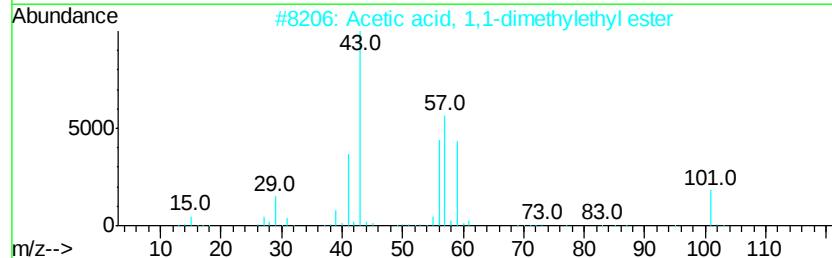
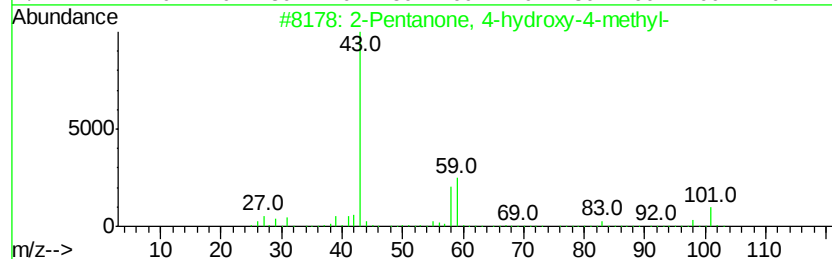
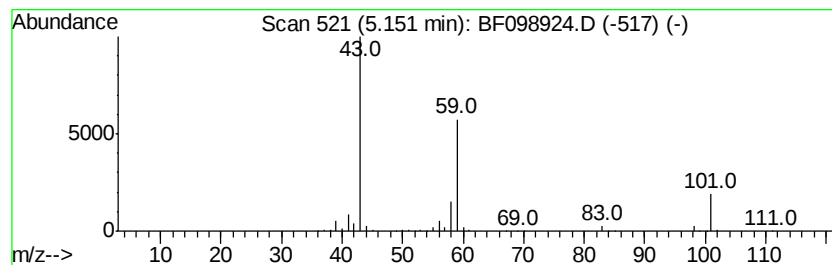
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	21.18 ng	983170	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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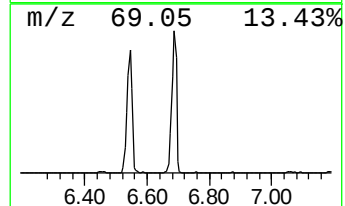
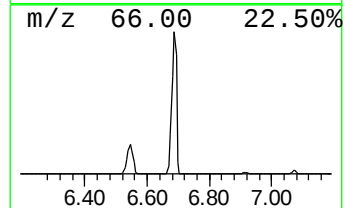
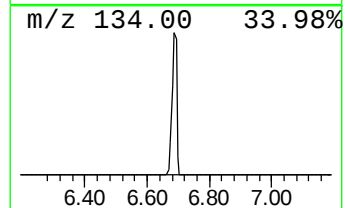
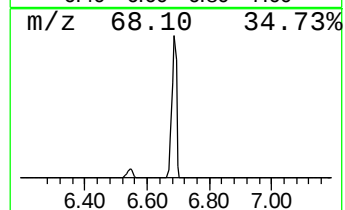
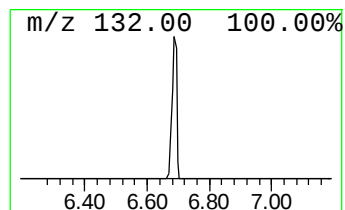
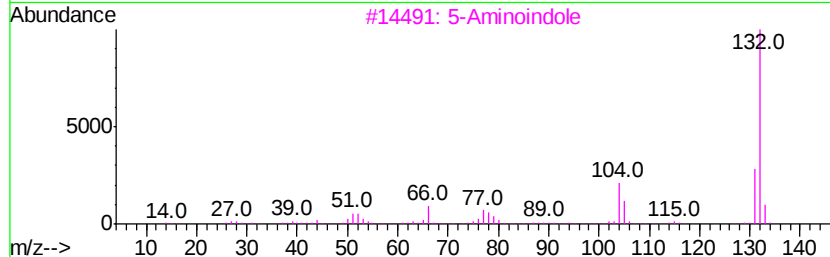
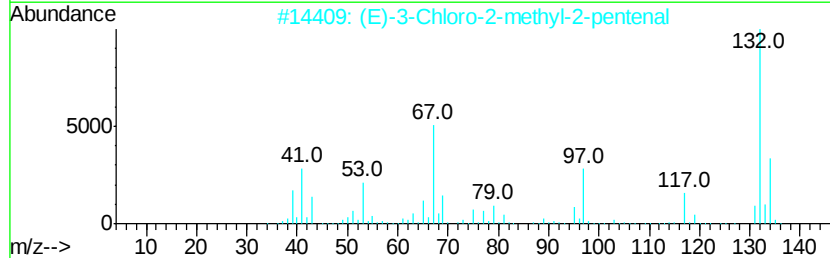
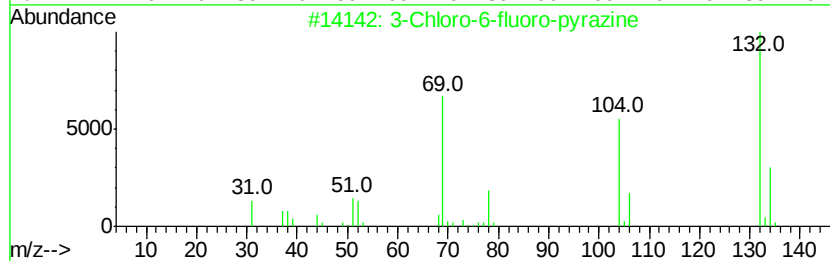
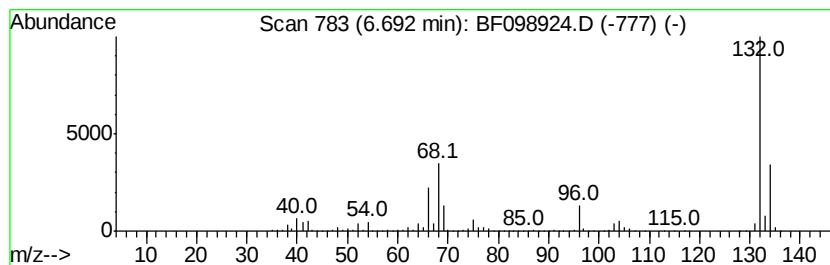
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	77.61 ng	3602530	1,4-Dichlorobenzene-d4	6.92

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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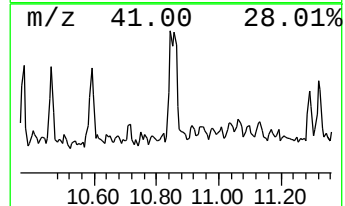
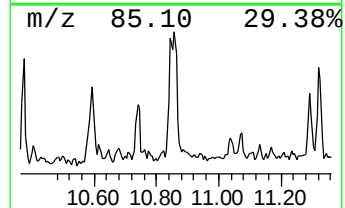
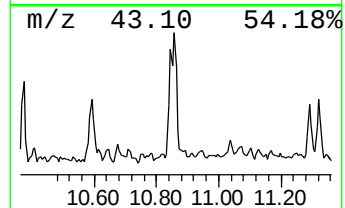
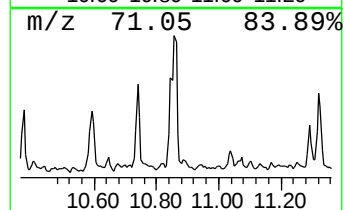
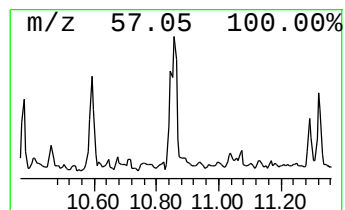
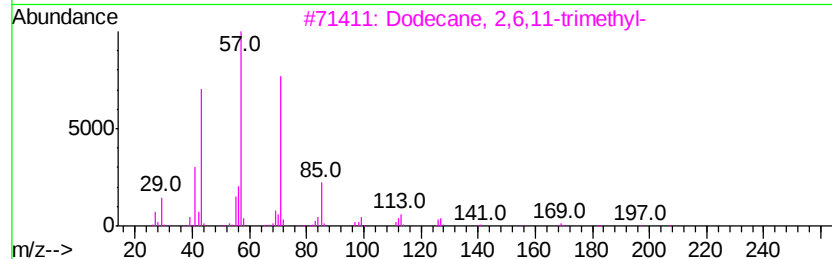
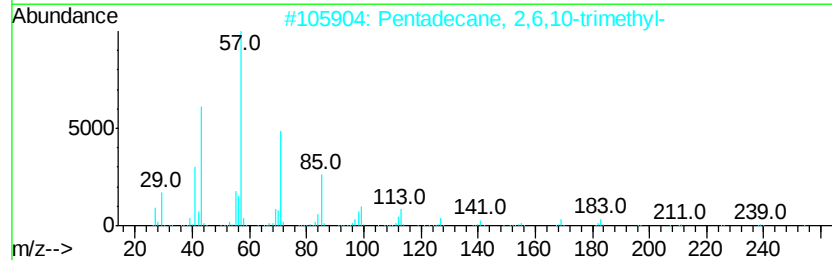
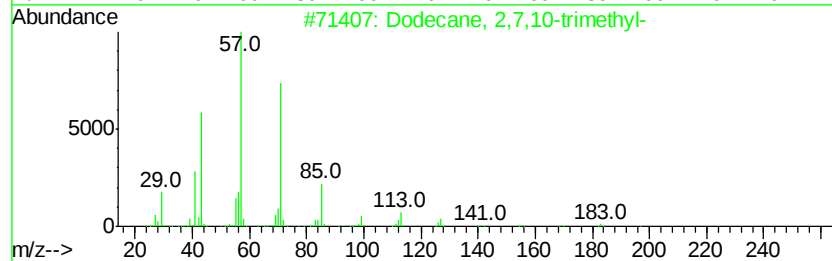
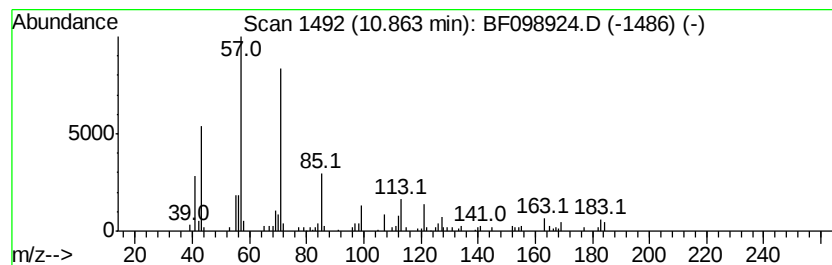
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecane, 2,7,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	4.59 ng	195458	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
4		Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
5		Tridecane	184	C13H28	000629-50-5	72



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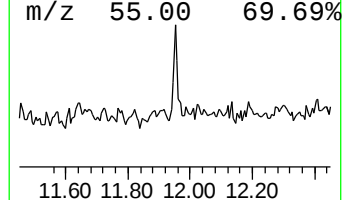
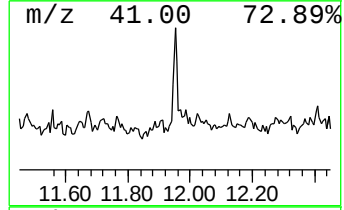
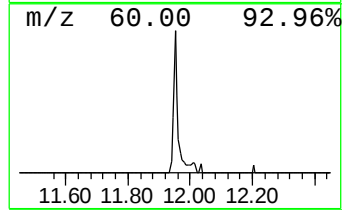
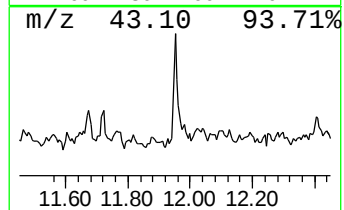
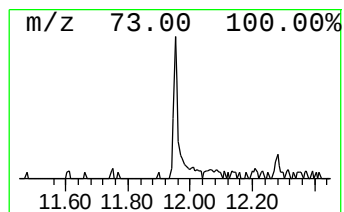
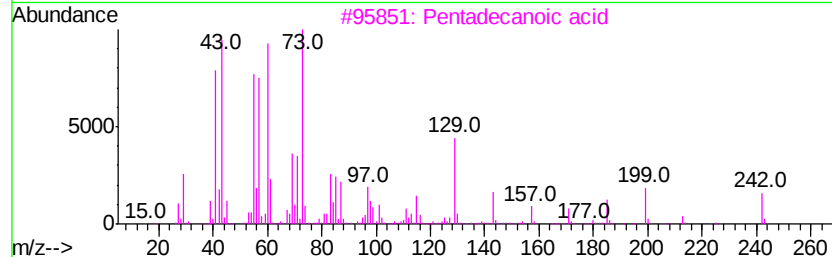
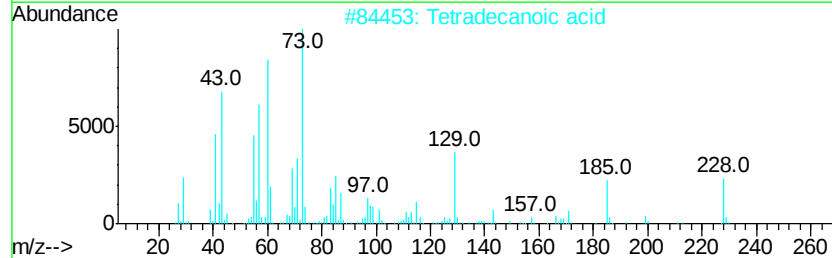
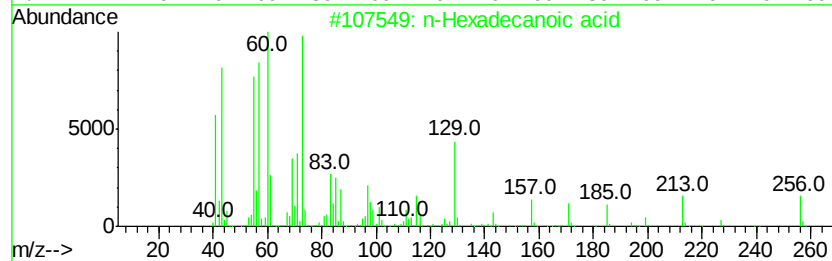
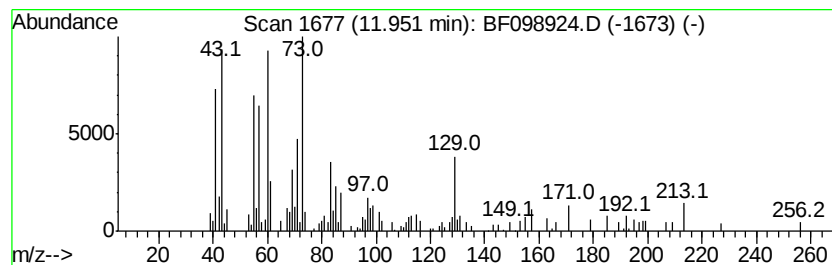
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.46 ng	104806	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		Trehalose	342	C12H22O11	000099-20-7	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098924.D
Acq On : 28 Sep 2017 23:24
Operator : SJ/JU
Sample : I5488-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-D

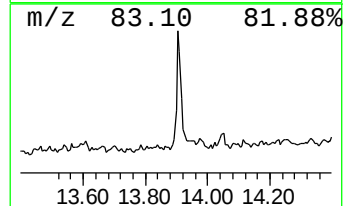
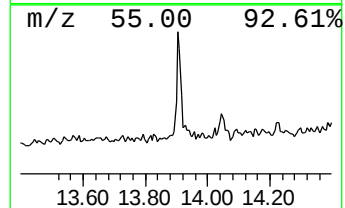
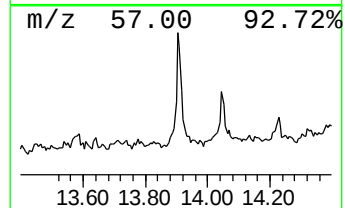
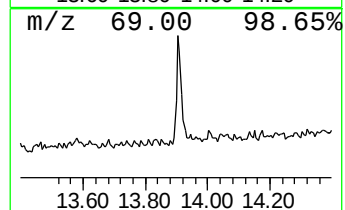
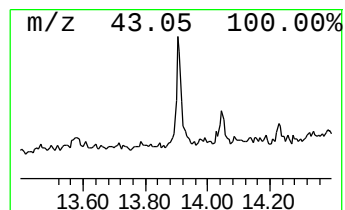
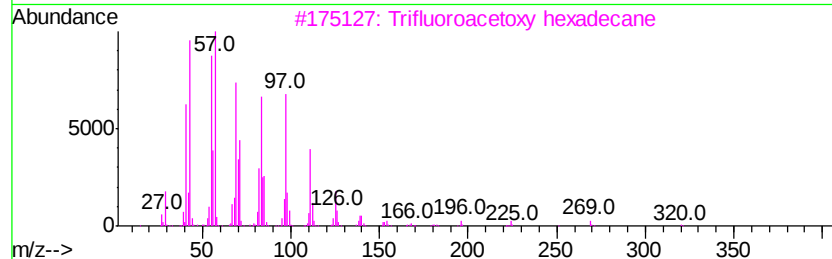
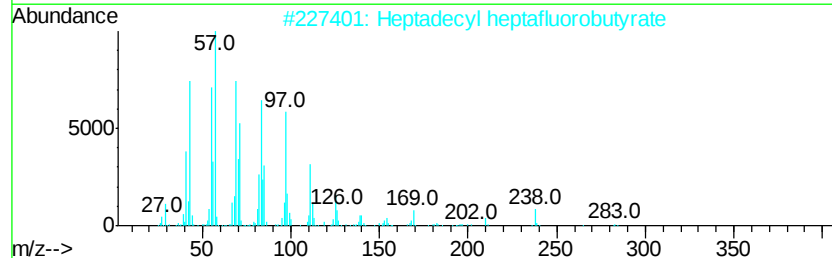
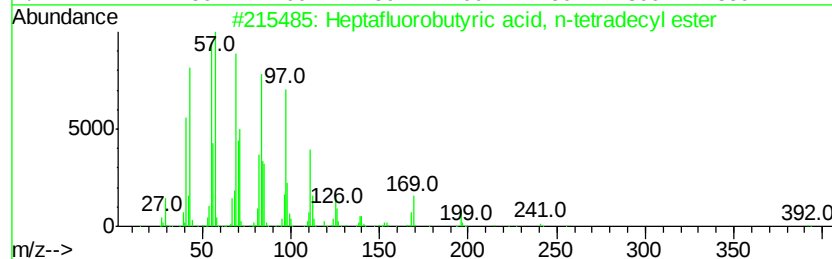
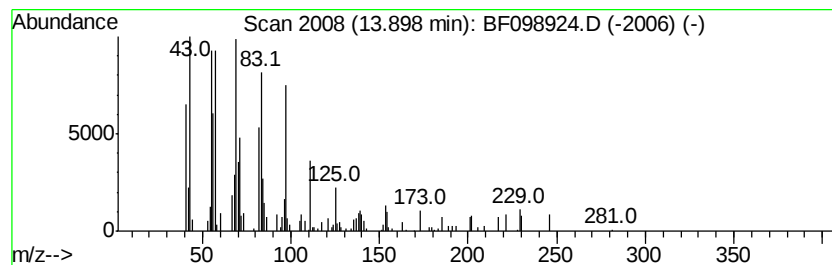
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutyric acid, n-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.54 ng	171239	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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Sample : I5488-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-D

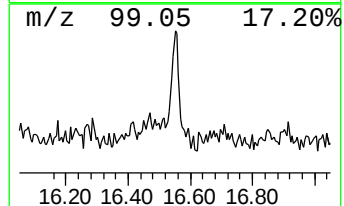
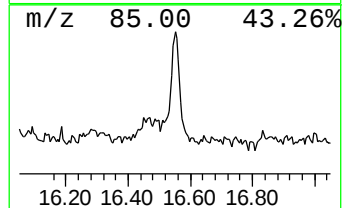
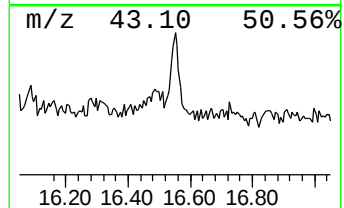
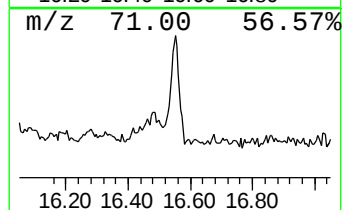
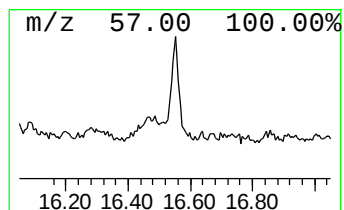
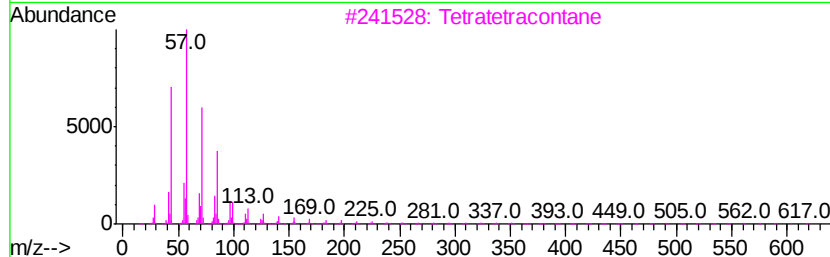
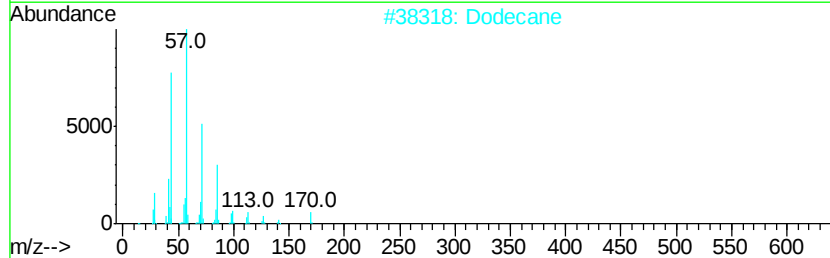
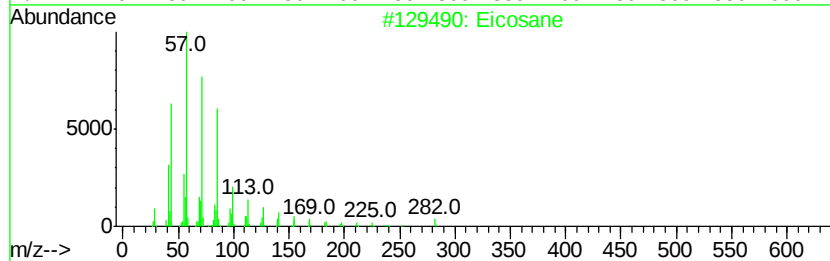
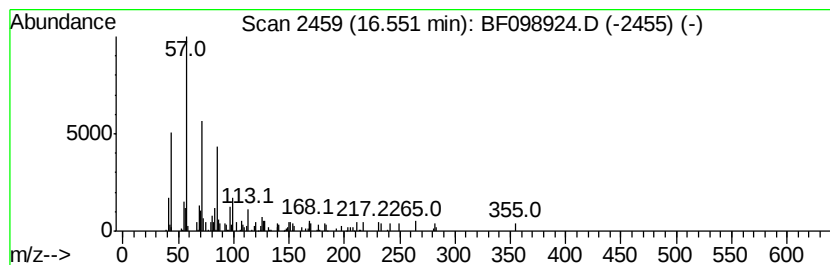
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.29 ng	94755	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	81
2	Dodecane		170	C12H26	000112-40-3	68
3	Tetratetracontane		619	C44H90	007098-22-8	68
4	Octacosane		394	C28H58	000630-02-4	68
5	Hexacosane		366	C26H54	000630-01-3	64



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Sample : I5488-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.25	5.9	ng	272009	1	6.92	928428	20.0
2-Pentanone, 4-hy...	5.15	21.2	ng	983170	1	6.92	928428	20.0
unknown6.69	6.69	77.6	ng	3602530	1	6.92	928428	20.0
Dodecane, 2,7,10-...	10.86	4.6	ng	195458	4	11.44	850875	20.0
n-Hexadecanoic acid	11.95	2.5	ng	104806	4	11.44	850875	20.0
Heptafluorobutyri...	13.90	4.5	ng	171239	5	14.08	754802	20.0
Eicosane	16.55	2.3	ng	94755	6	15.57	829177	20.0