

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
 Data File : BF108648.D
 Acq On : 30 Aug 2018 18:56
 Operator : JU/SJ
 Sample : J4702-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-039

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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	5.237	490	493	501	rBV2	19468	34889	1.80%	0.197%
2	5.648	558	563	594	rBV	192433	967401	49.82%	5.450%
3	6.642	728	732	751	rBV	396460	1209632	62.29%	6.815%
4	6.772	751	754	790	rVV	788811	1661985	85.58%	9.363%
5	7.001	790	793	815	rVV	240794	505952	26.05%	2.850%
6	7.154	815	819	841	rVV	704461	1062149	54.70%	5.984%
7	7.566	885	889	911	rBV	407719	891650	45.92%	5.023%
8	8.283	1007	1011	1041	rBV	403657	685568	35.30%	3.862%
9	9.219	1165	1170	1178	rBV3	11644	23572	1.21%	0.133%
10	9.354	1189	1193	1207	rVV	1363199	1699099	87.50%	9.572%
11	9.448	1207	1209	1223	rVB	60417	87421	4.50%	0.493%
12	9.748	1256	1260	1271	rBV	107653	152485	7.85%	0.859%
13	10.042	1306	1310	1325	rBV	696203	826577	42.56%	4.657%
14	10.836	1441	1445	1457	rBV	932344	1230496	63.36%	6.932%
15	11.536	1561	1564	1579	rBV	717049	921308	47.44%	5.191%
16	11.766	1597	1603	1606	rBV7	15992	32564	1.68%	0.183%
17	11.866	1616	1620	1624	rBV2	24962	30819	1.59%	0.174%
18	12.036	1646	1649	1653	rBV	52139	66512	3.43%	0.375%
19	12.077	1653	1656	1661	rVB	41308	50770	2.61%	0.286%
20	12.589	1738	1743	1751	rVB3	28471	54906	2.83%	0.309%
21	12.966	1804	1807	1815	rVB5	14899	25404	1.31%	0.143%
22	13.118	1829	1833	1844	rBV	2025177	1941921	100.00%	10.940%
23	13.318	1864	1867	1869	rBV2	22649	23076	1.19%	0.130%
24	13.548	1903	1906	1909	rBV3	27963	25219	1.30%	0.142%
25	13.660	1923	1925	1930	rBV4	21304	27435	1.41%	0.155%
26	14.012	1979	1985	1996	rBV3	140932	291176	14.99%	1.640%
27	14.189	2011	2015	2023	rBV	676786	768529	39.58%	4.330%
28	14.307	2032	2035	2038	rBV2	38558	36075	1.86%	0.203%
29	14.612	2084	2087	2091	rBV	87808	76427	3.94%	0.431%
30	14.936	2138	2142	2146	rBV	153876	168458	8.67%	0.949%
31	15.018	2154	2156	2161	rVB2	34038	38098	1.96%	0.215%
32	15.295	2199	2203	2213	rVB	316020	382867	19.72%	2.157%
33	15.707	2268	2273	2276	rBV	256190	365218	18.81%	2.058%
34	15.748	2276	2280	2290	rVB	451456	702287	36.16%	3.957%

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ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
FK-PS-01-039

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	16.171	2347	2352	2359	rVB	200899	329973	16.99%	1.859%
36	16.718	2440	2445	2451	rBV	85433	151411	7.80%	0.853%
37	17.989	2655	2661	2677	rVB	53450	200516	10.33%	1.130%

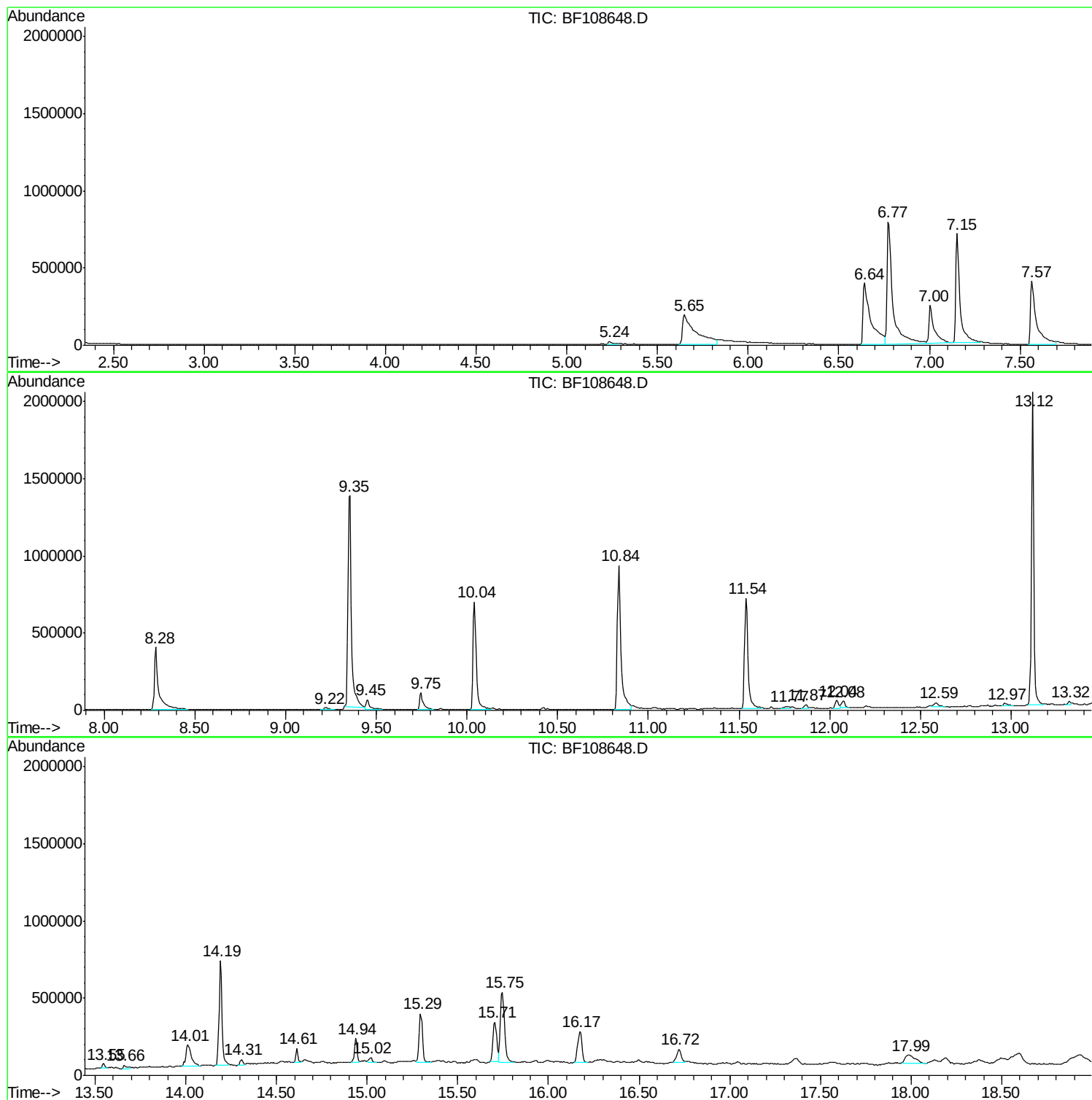
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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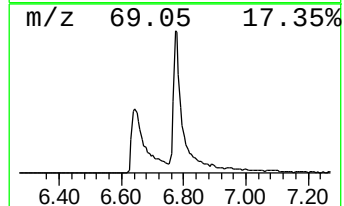
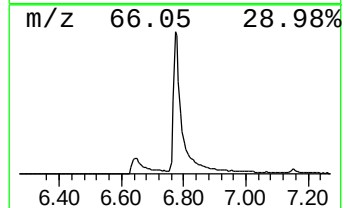
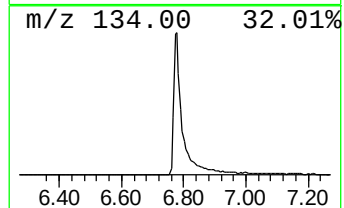
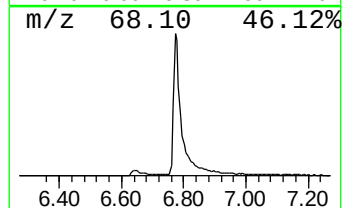
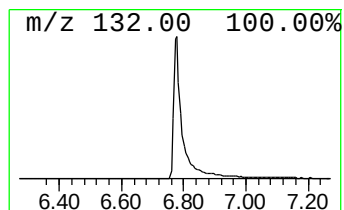
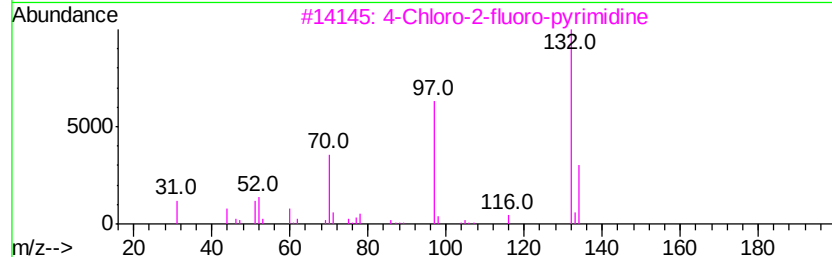
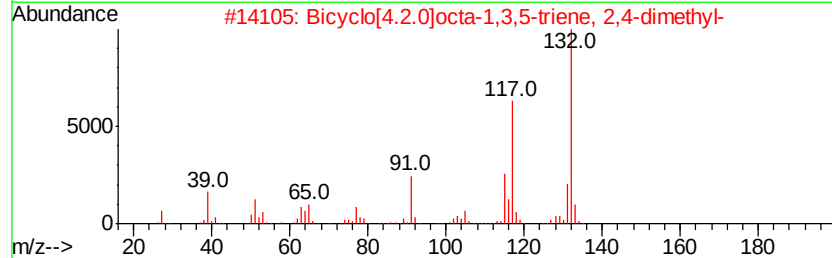
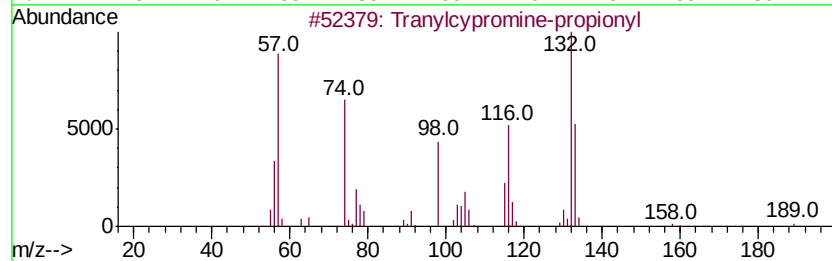
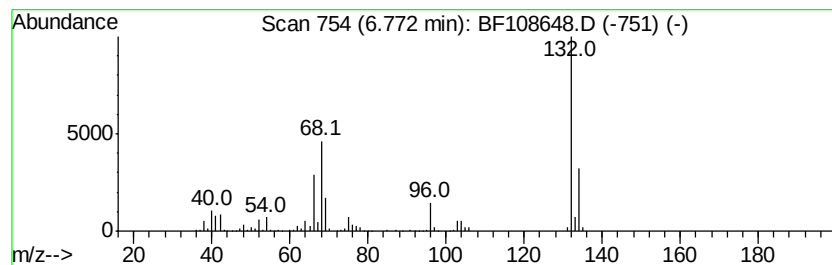
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	65.70 ng	1661990	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypropromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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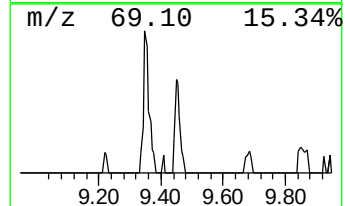
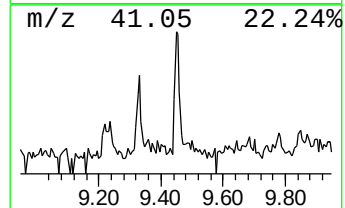
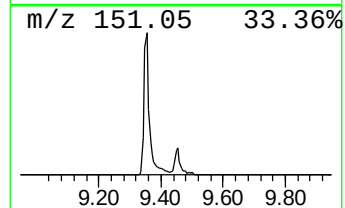
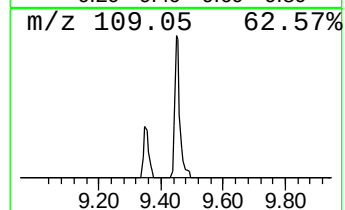
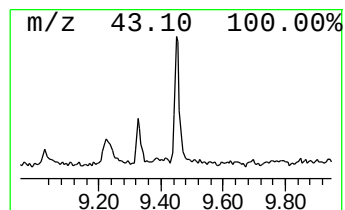
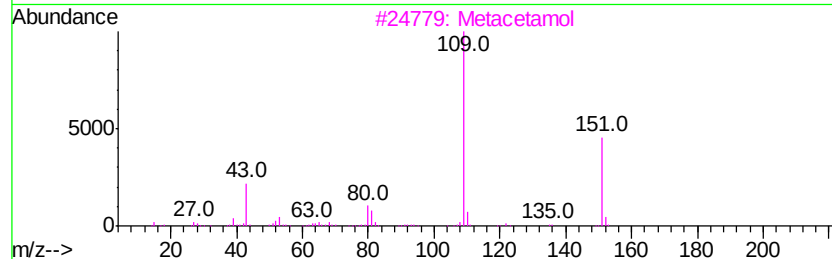
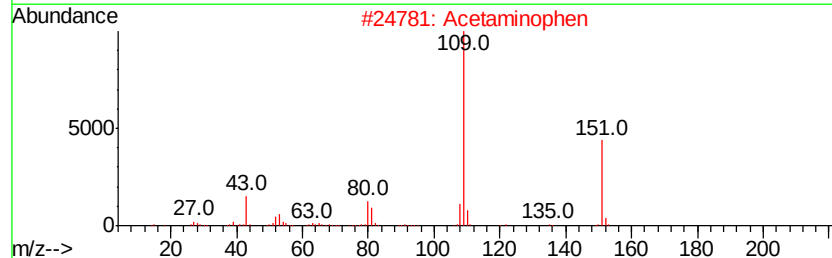
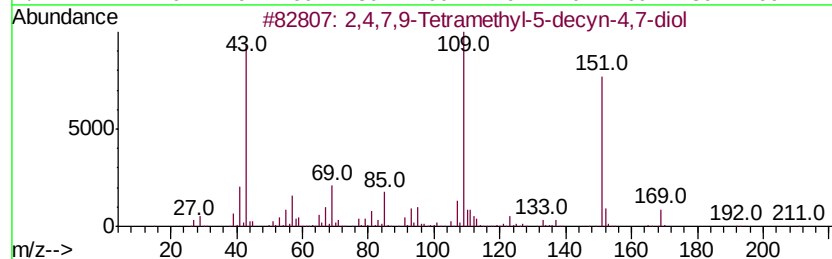
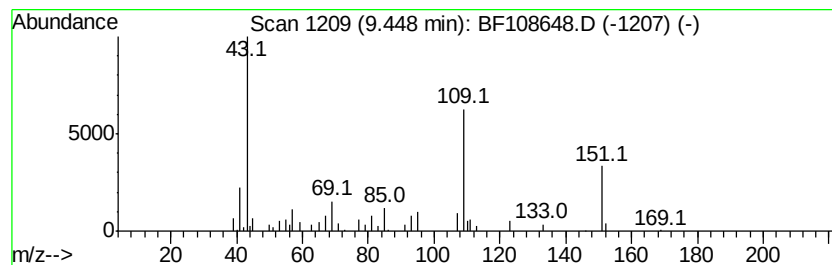
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	2.12 ng	87421	Acenaphthene-d10	10.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	83		
2	Acetaminophen	151	C8H9NO2	000103-90-2	49		
3	Metacetamol	151	C8H9NO2	000621-42-1	47		
4	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	45		
5	2-Cyclohexen-1-ol, 2-methyl-5-(1...	152	C10H16O	001197-06-4	43		



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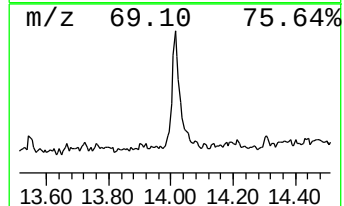
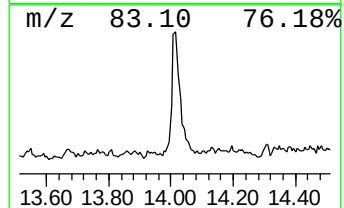
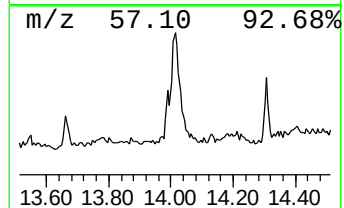
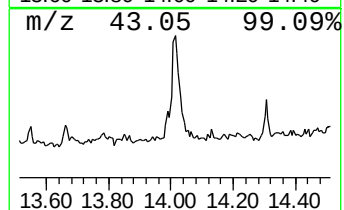
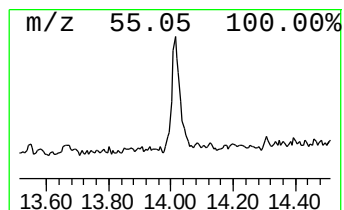
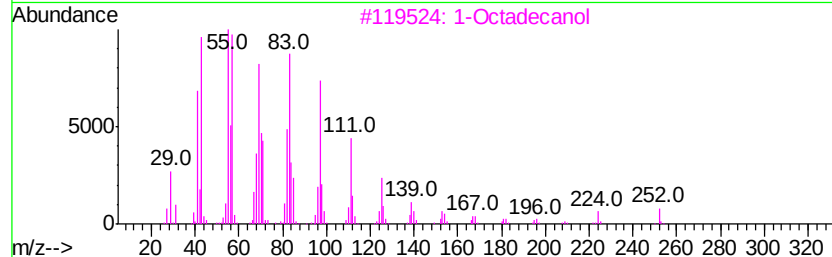
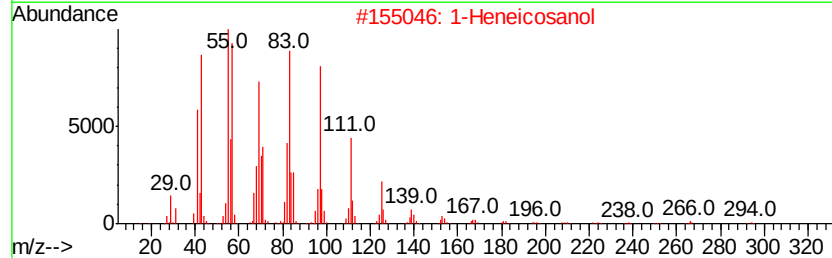
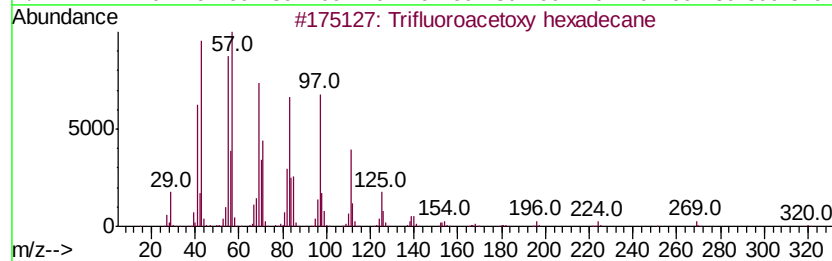
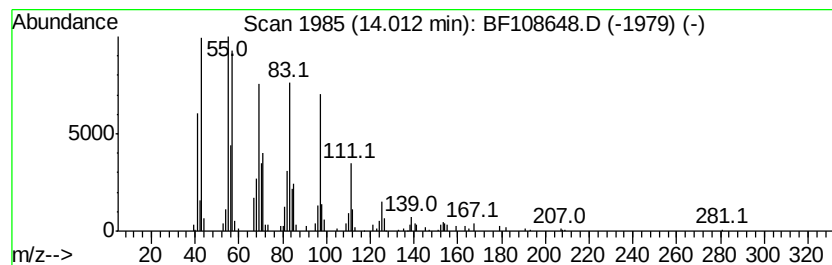
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	7.58 ng	291176	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		1-Octadecanol	270	C18H38O	000112-92-5	94
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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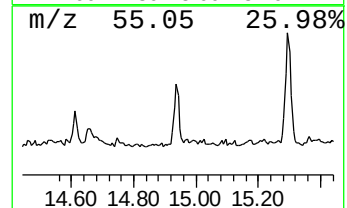
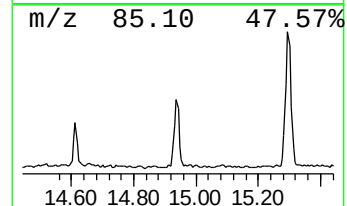
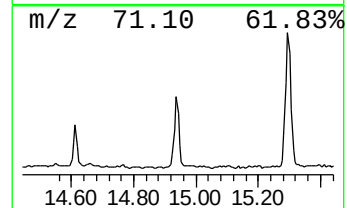
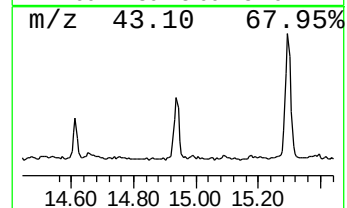
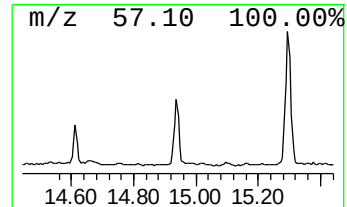
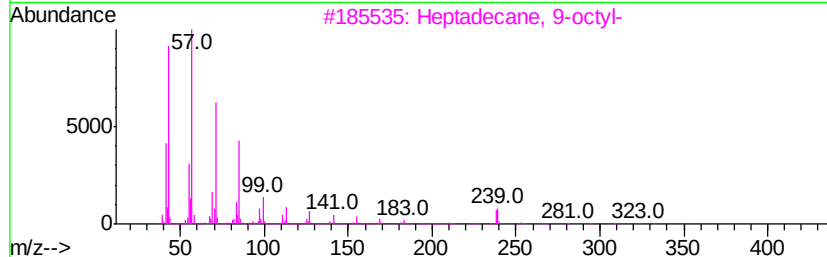
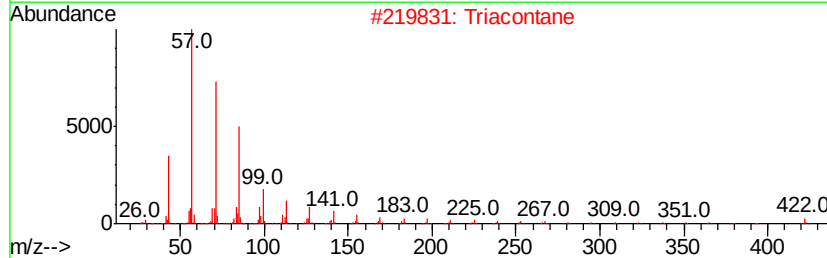
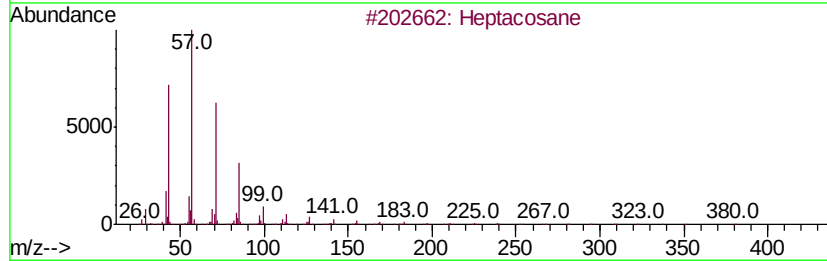
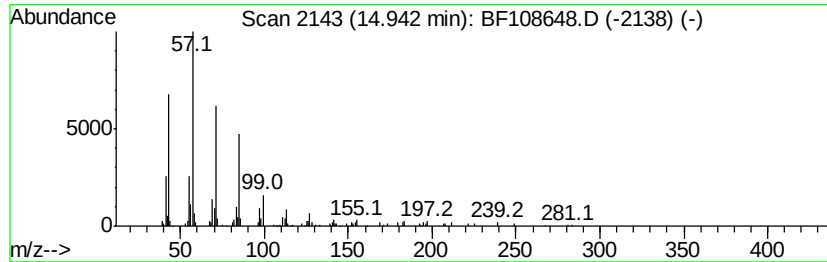
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	4.38 ng	168458	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Triacontane		422	C30H62	000638-68-6	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Eicosane		282	C20H42	000112-95-8	91
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	91



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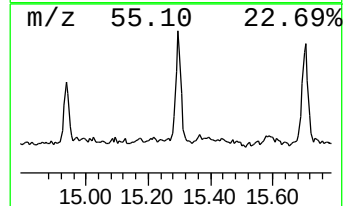
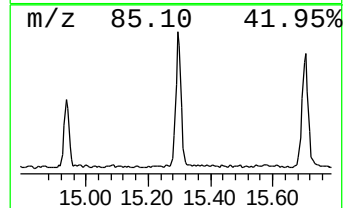
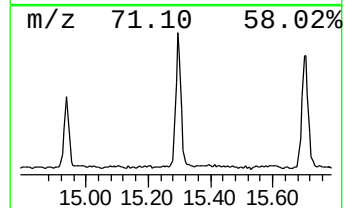
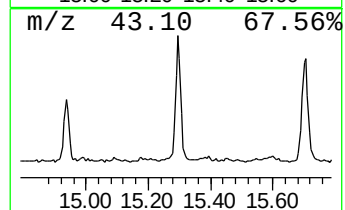
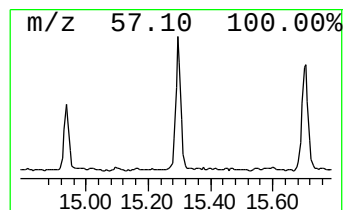
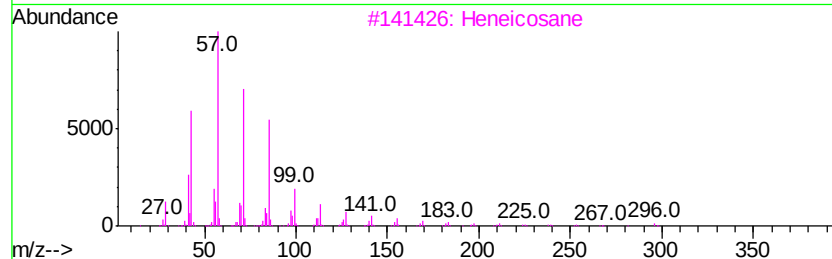
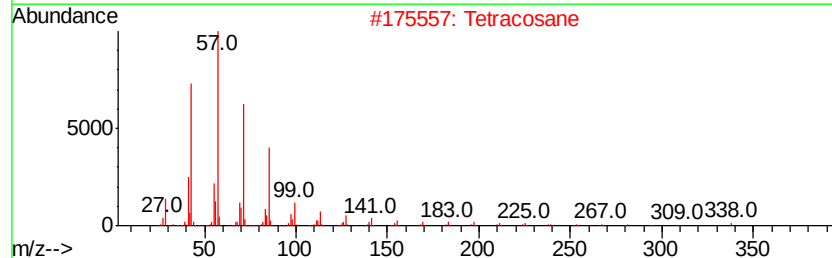
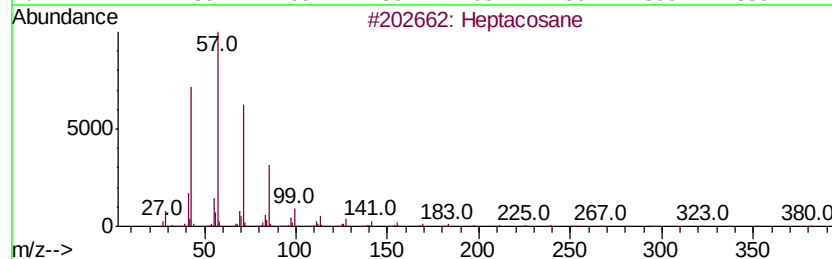
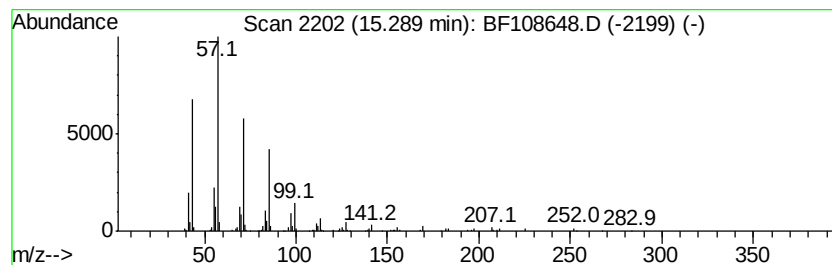
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	10.90 ng	382867	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Tetracosane	338	C24H50	000646-31-1	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Docosane	310	C22H46	000629-97-0	87



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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-039

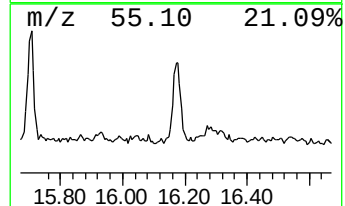
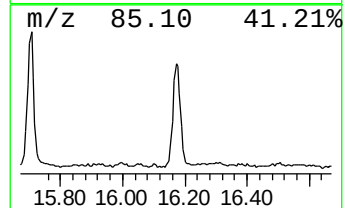
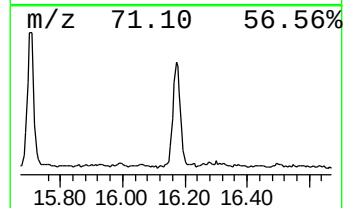
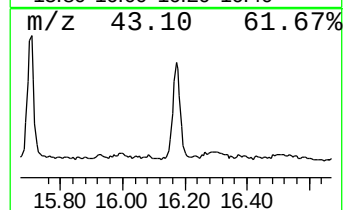
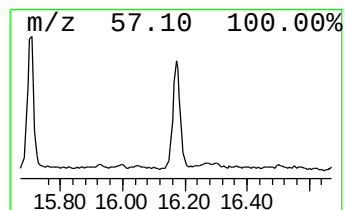
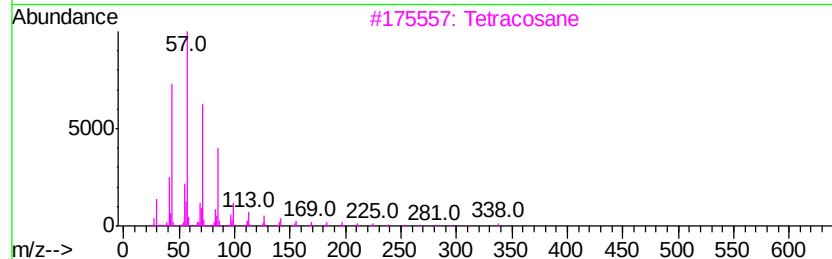
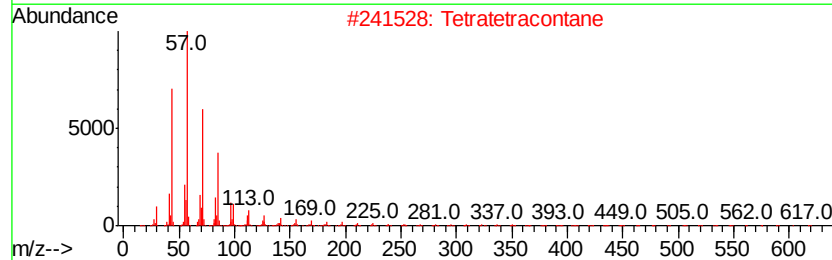
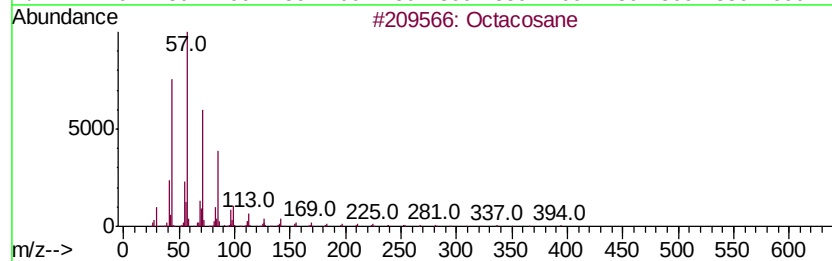
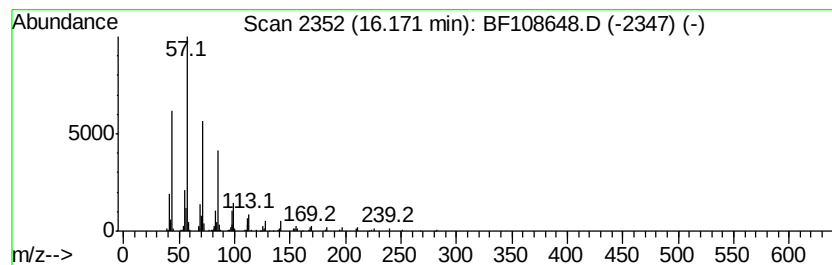
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	9.40 ng	329973	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexatriacontane	507	C36H74	000630-06-8	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108648.D
Acq On : 30 Aug 2018 18:56
Operator : JU/SJ
Sample : J4702-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-039

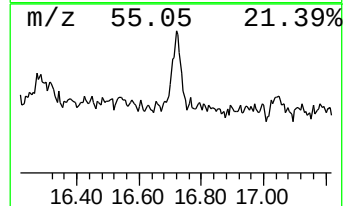
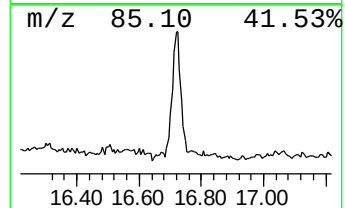
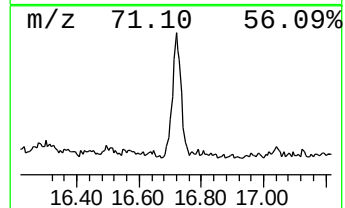
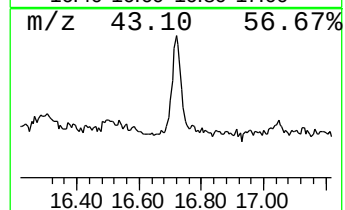
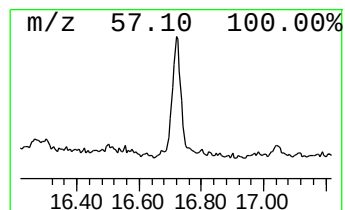
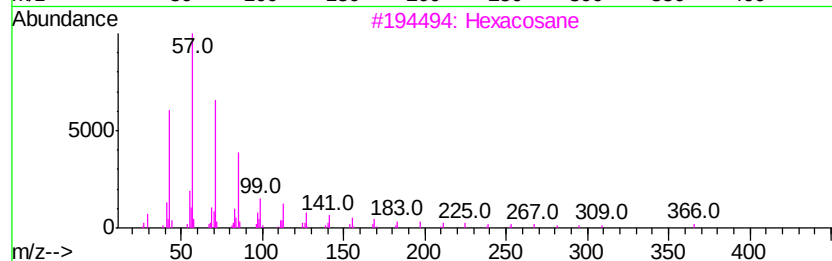
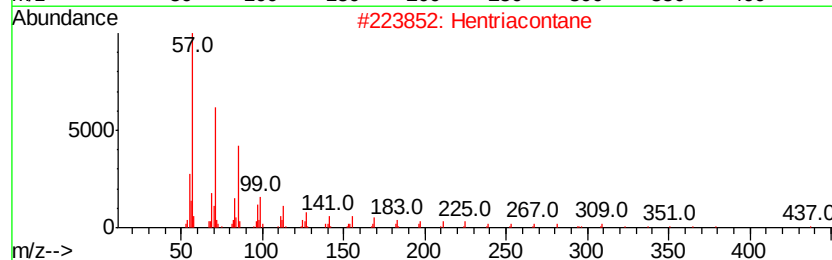
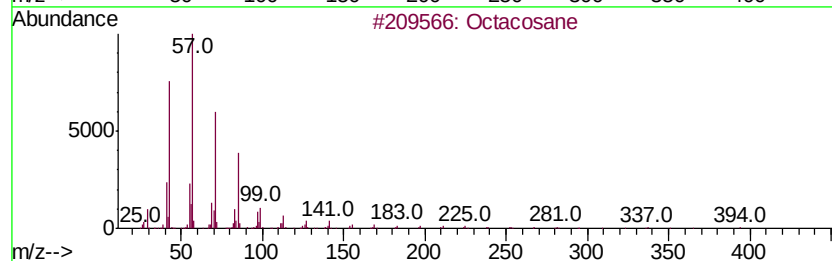
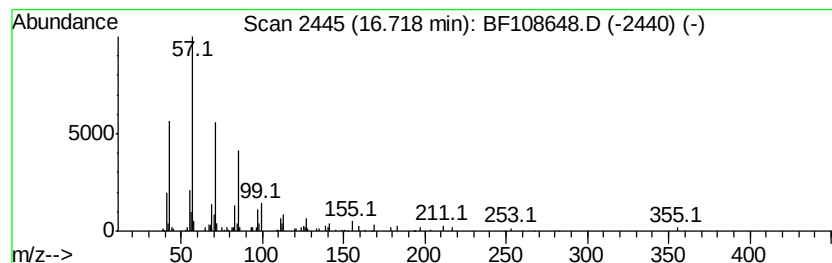
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane, 11-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	4.31 ng	151411	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108648.D
Acq On : 30 Aug 2018 18:56
Operator : JU/SJ
Sample : J4702-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

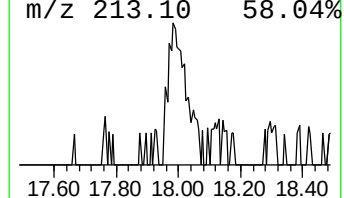
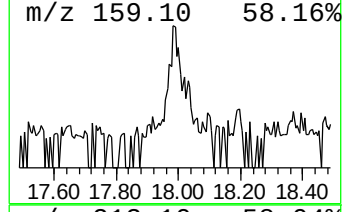
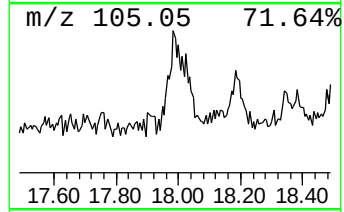
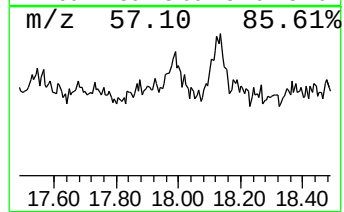
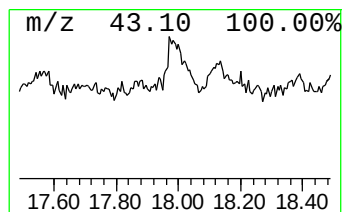
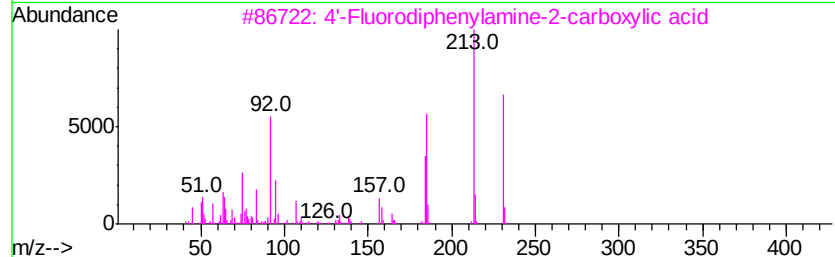
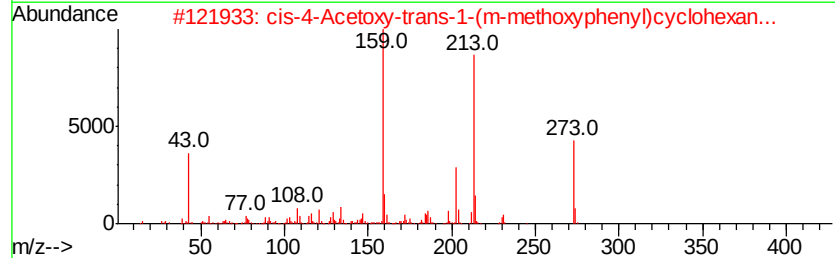
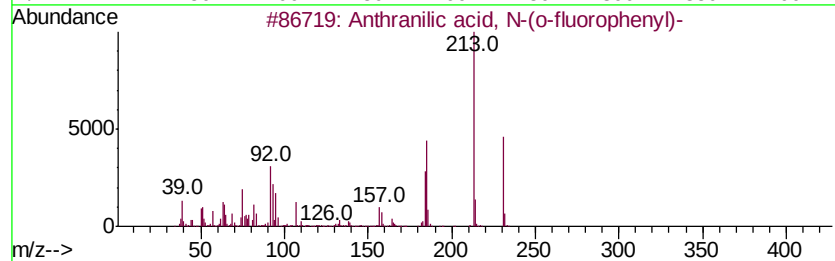
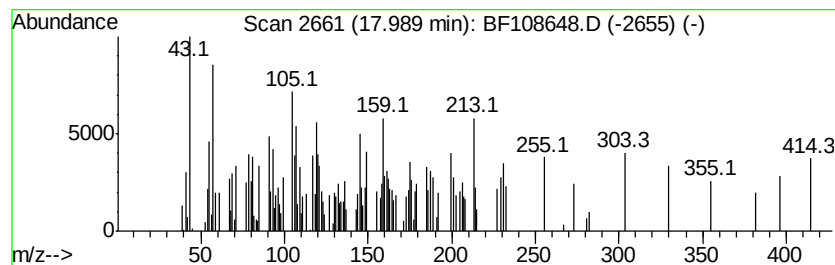
Instrument :
BNA_F
ClientSampleId :
FK-PS-01-039

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.99	5.71 ng	200516	Perylene-d12	15.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthranilic acid, N-(o-fluorophe...	231	C13H10FN02	000054-58-0	11
2	cis-4-Acetoxy-trans-1-(m-methoxy...	273	C16H19N03	1000241-10-4	10
3	4'-Fluorodiphenylamine-2-carboxv...	231	C13H10FN02	000054-60-4	10
4	2-(p-Nitrobenzyl)pyridine	214	C12H10N2O2	000620-87-1	9
5	Dibenzofuran, 2-nitro-	213	C12H7N03	020927-95-1	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083018\
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Acq On : 30 Aug 2018 18:56
Operator : JU/SJ
Sample : J4702-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-039

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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
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2,4,7,9-Tetrameth...	9.45	2.1	ng	87421	3	10.04	826577	20.0
Trifluoroacetoxy ...	14.01	7.6	ng	291176	5	14.19	768529	20.0
Heptacosane	14.94	4.4	ng	168458	5	14.19	768529	20.0
Tetracosane	15.29	10.9	ng	382867	6	15.75	702287	20.0
Octacosane	16.17	9.4	ng	329973	6	15.75	702287	20.0
Docosane, 11-butyl-	16.72	4.3	ng	151411	6	15.75	702287	20.0
unknown17.99	17.99	5.7	ng	200516	6	15.75	702287	20.0