

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
 Data File : BF100150.D
 Acq On : 3 Nov 2017 22:20
 Operator : SJ/JU
 Sample : I6294-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N48971

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-BF102317.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	4.616	427	430	442	rBV	26636	50528	1.94%	0.281%
2	4.987	490	493	509	rBV	79593	129334	4.96%	0.720%
3	5.316	545	549	556	rBV	30496	42501	1.63%	0.237%
4	5.392	559	562	583	rBV	882617	1167793	44.79%	6.500%
5	6.416	734	736	751	rBV	543427	787266	30.20%	4.382%
6	6.545	754	758	767	rVB	1996846	1984160	76.10%	11.044%
7	6.769	793	796	805	rBV	554307	515551	19.77%	2.870%
8	6.922	818	822	841	rBV	1911403	1794968	68.85%	9.991%
9	7.316	885	889	890	rBV	37801	32256	1.24%	0.180%
10	7.345	890	894	912	rVB	1400992	1432380	54.94%	7.973%
11	8.051	1011	1014	1028	rBV	795184	725679	27.83%	4.039%
12	8.627	1109	1112	1120	rBV	91047	83194	3.19%	0.463%
13	9.127	1192	1197	1200	rBV	2825809	2607194	100.00%	14.512%
14	9.804	1308	1312	1322	rVB	897505	767522	29.44%	4.272%
15	10.604	1444	1448	1461	rBV	1316474	1309785	50.24%	7.291%
16	11.298	1562	1566	1573	rBV	771693	674123	25.86%	3.752%
17	11.810	1651	1653	1658	rBV	73253	72120	2.77%	0.401%
18	12.598	1784	1787	1791	rBV	43256	49160	1.89%	0.274%
19	12.768	1812	1816	1826	rBV	579937	610346	23.41%	3.397%
20	12.880	1831	1835	1838	rBV	1943700	1818096	69.73%	10.120%
21	13.757	1981	1984	1990	rVB3	58062	68050	2.61%	0.379%
22	13.951	2014	2017	2024	rVB	440731	422131	16.19%	2.350%
23	14.427	2096	2098	2102	rVB4	26736	27265	1.05%	0.152%
24	15.303	2244	2247	2252	rVB7	23577	29153	1.12%	0.162%
25	15.409	2261	2265	2273	rVB	332814	431334	16.54%	2.401%
26	15.774	2324	2327	2333	rVB2	23366	32386	1.24%	0.180%
27	16.021	2365	2369	2384	rVB3	41245	88613	3.40%	0.493%
28	16.250	2404	2408	2421	rVB7	22982	68697	2.63%	0.382%
29	16.433	2434	2439	2445	rVB	46462	77905	2.99%	0.434%
30	16.809	2500	2503	2510	rVB7	13923	27187	1.04%	0.151%
31	17.474	2610	2616	2622	rBV5	18697	38746	1.49%	0.216%

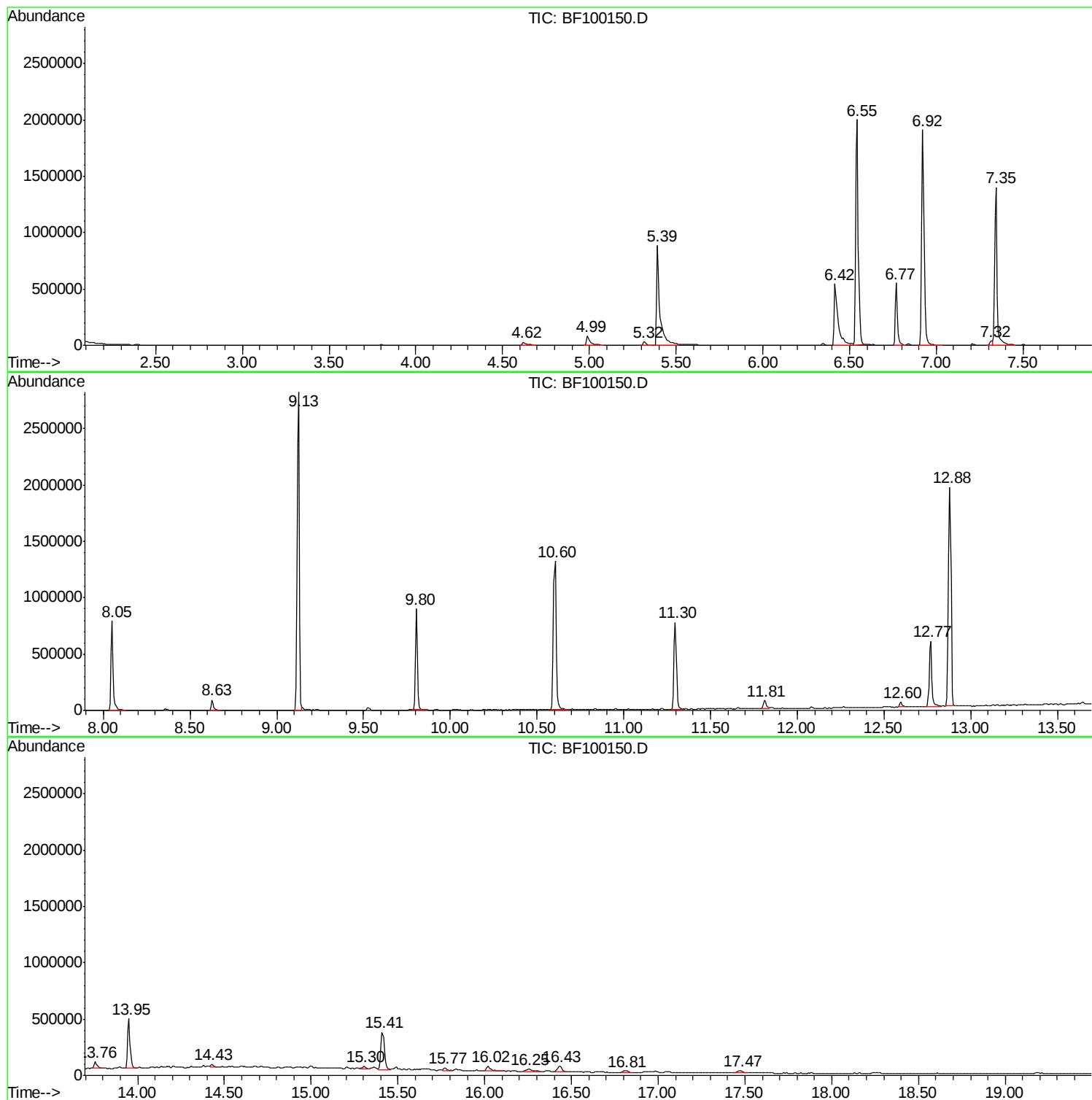
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ALS Vial : 21 Sample Multiplier: 1

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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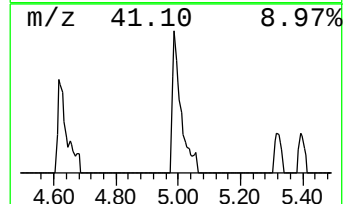
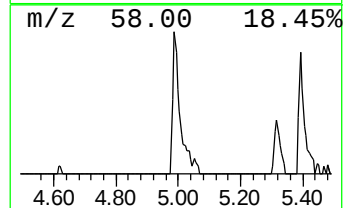
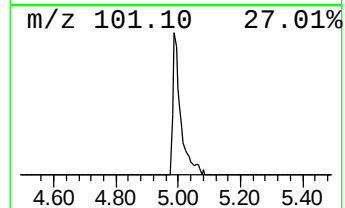
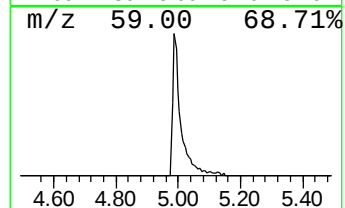
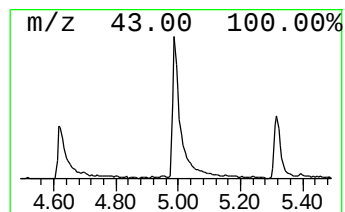
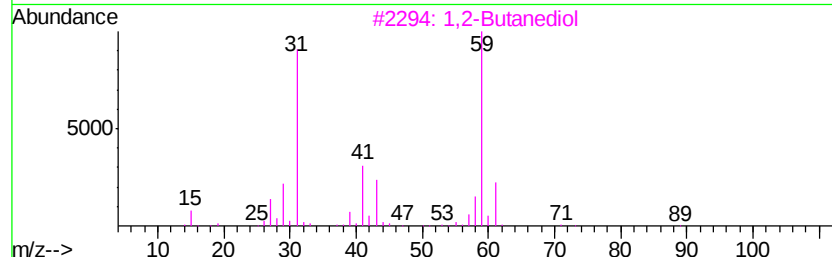
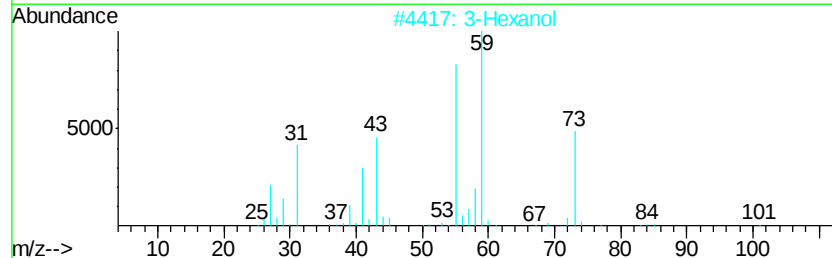
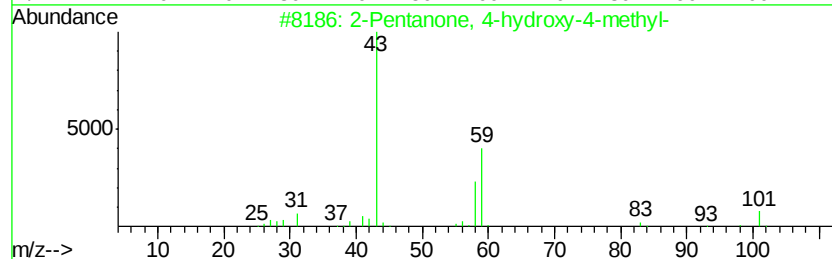
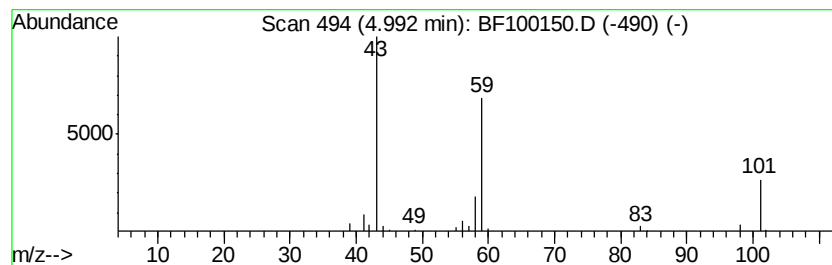
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	5.02 ng	129334	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol	102	C6H14O	000623-37-0	28
3			1,2-Butanediol	90	C4H10O2	000584-03-2	23
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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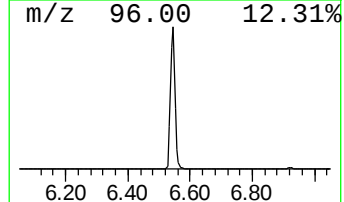
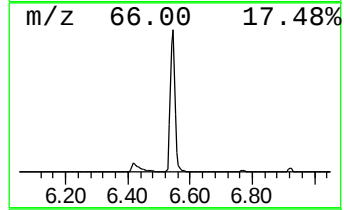
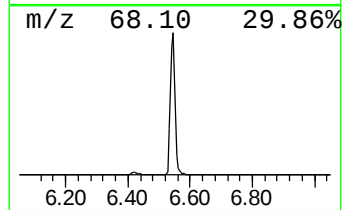
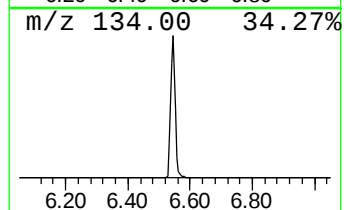
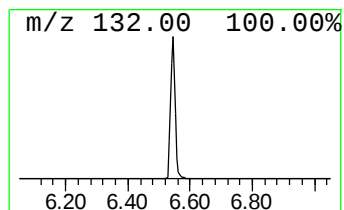
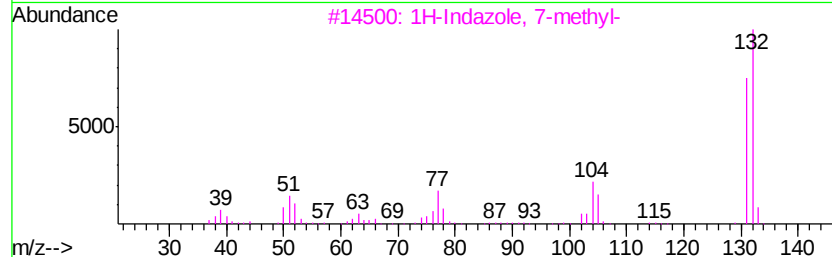
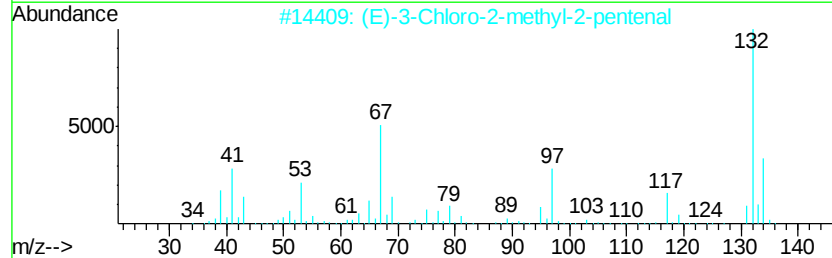
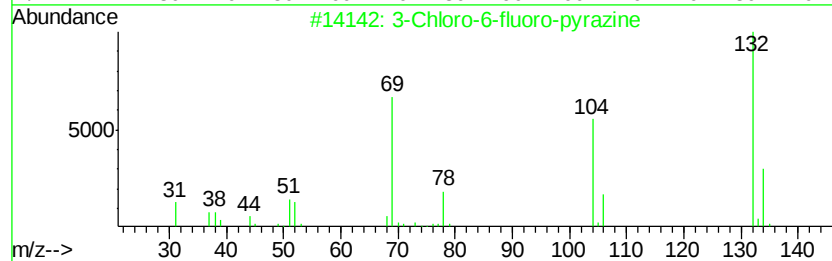
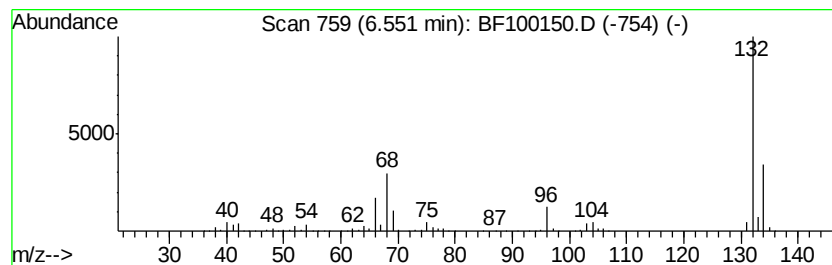
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	76.97 ng	1984160	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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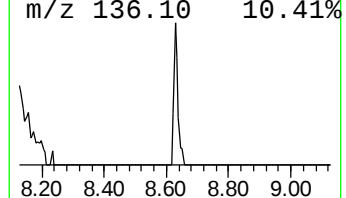
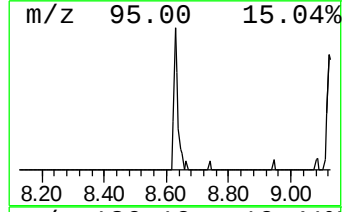
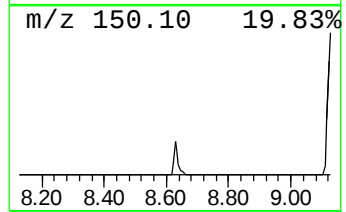
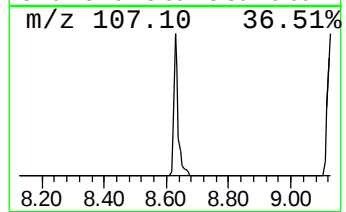
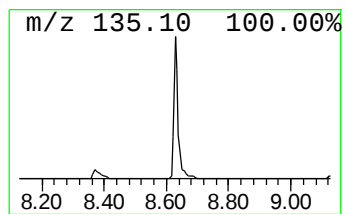
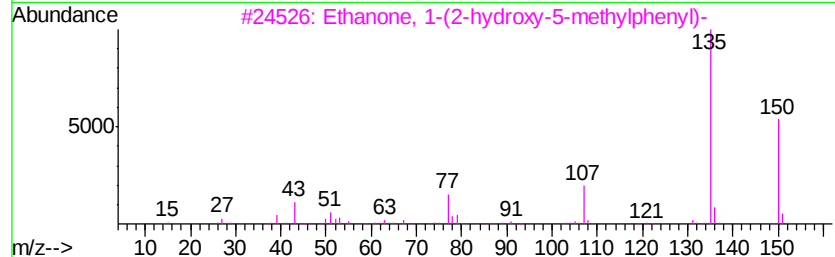
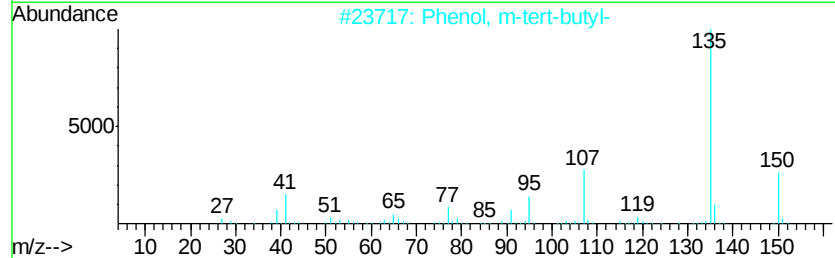
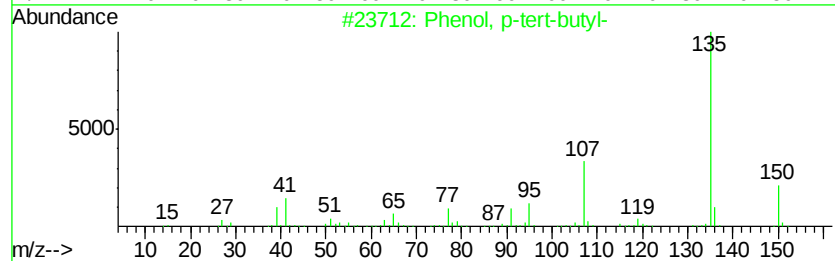
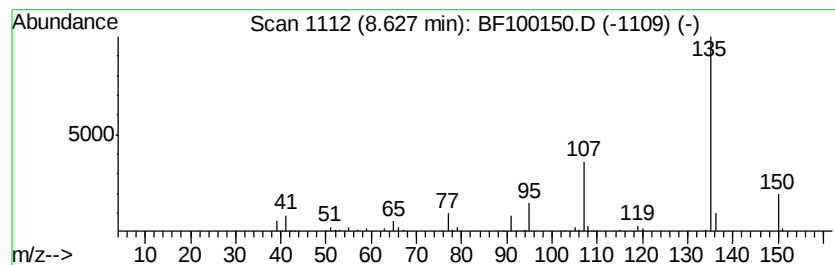
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Peak Number 4 Phenol, p-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.29 ng	83194	Naphthalene-d8	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
2		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	93
3		Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	64
4		ortho-Methoxyacetophenone	150	C9H10O2	000579-74-8	59
5		Benzene, 1-methoxy-4-(1-methylet...	150	C10H14O	004132-48-3	58



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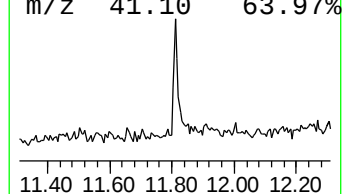
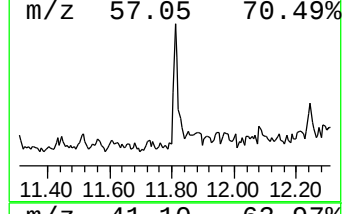
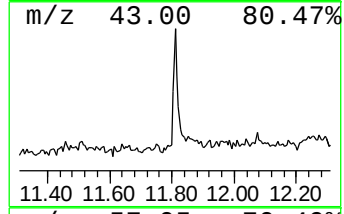
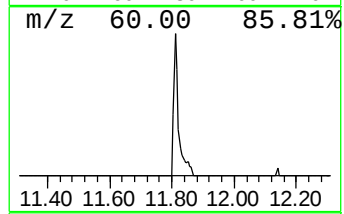
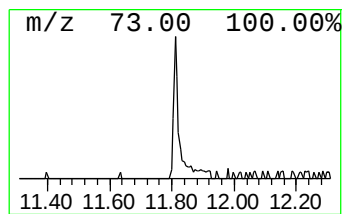
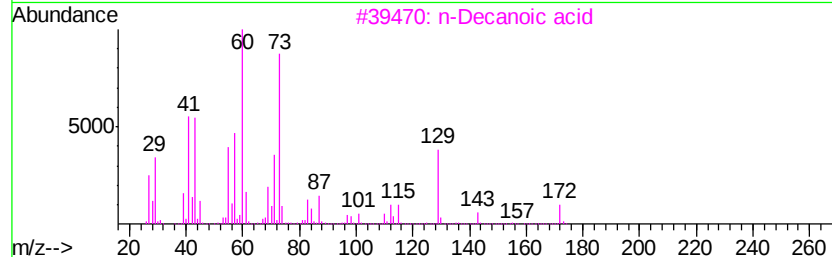
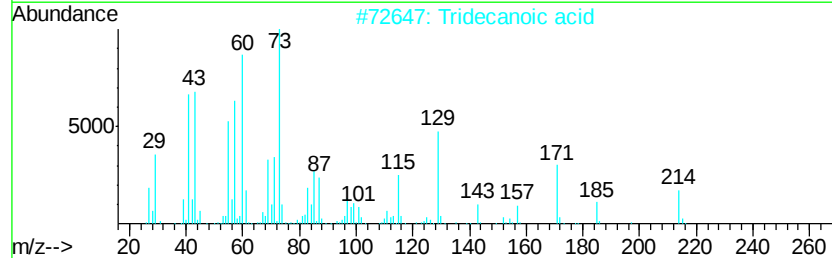
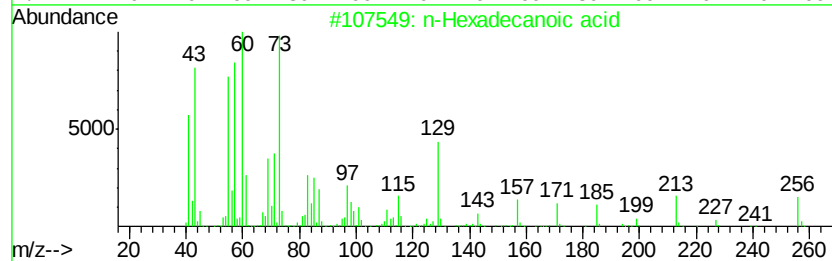
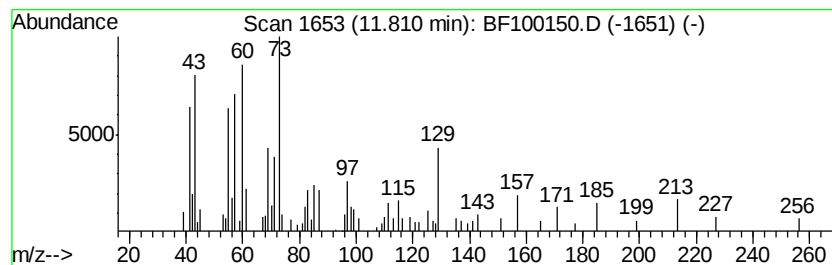
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	2.14 ng	72120	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Tridecanoic acid	214	C13H26O2	000638-53-9	80
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	15
5		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	11



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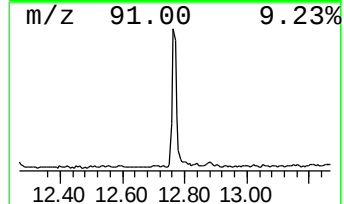
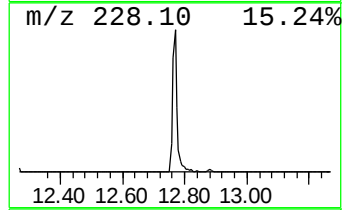
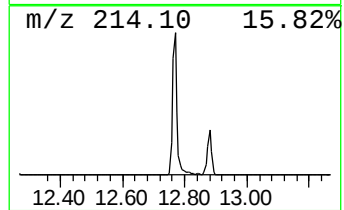
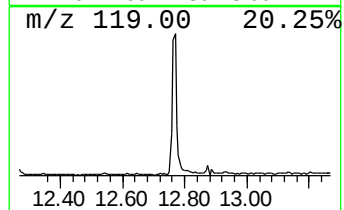
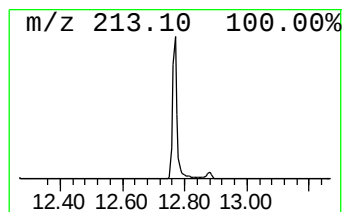
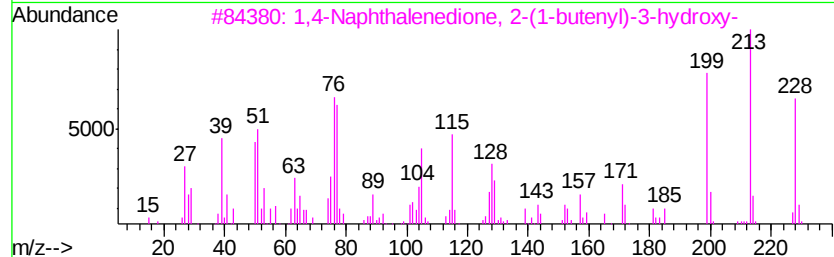
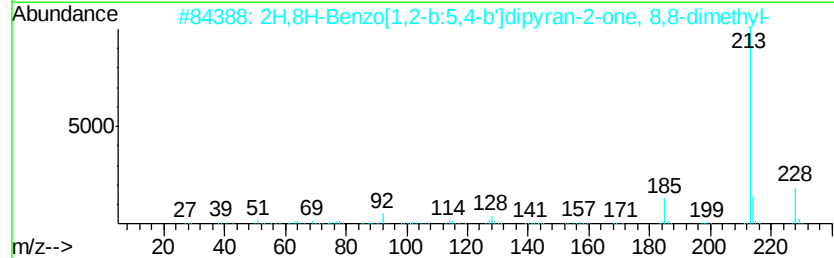
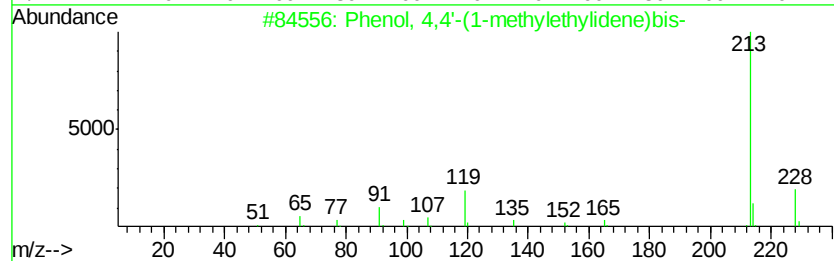
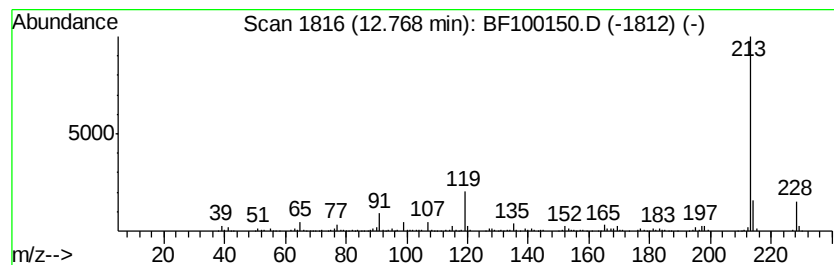
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Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	28.92 ng	610346	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	50
3		1,4-Naphthalenedione, 2-(1-buten...	228	C14H12O3	029366-43-6	47
4		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	40
5		2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	40



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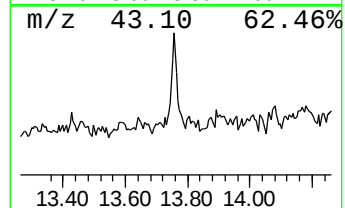
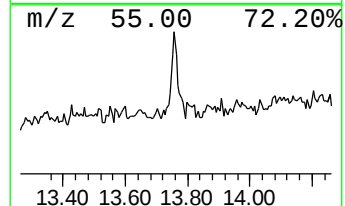
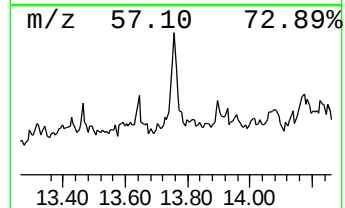
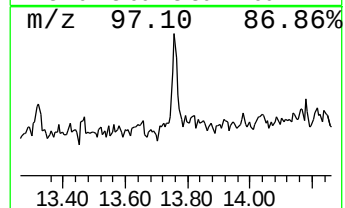
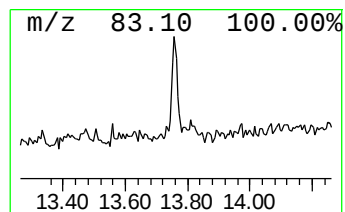
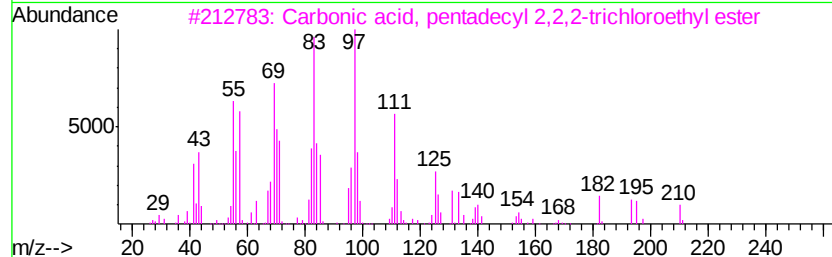
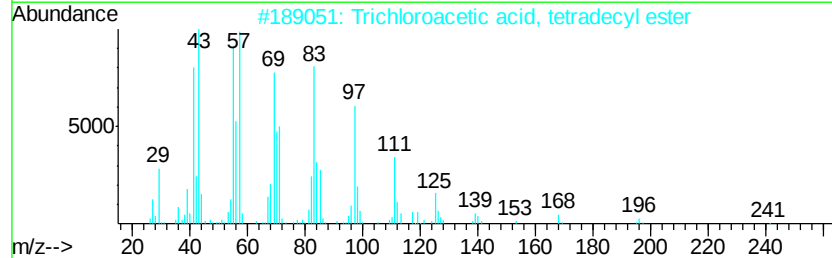
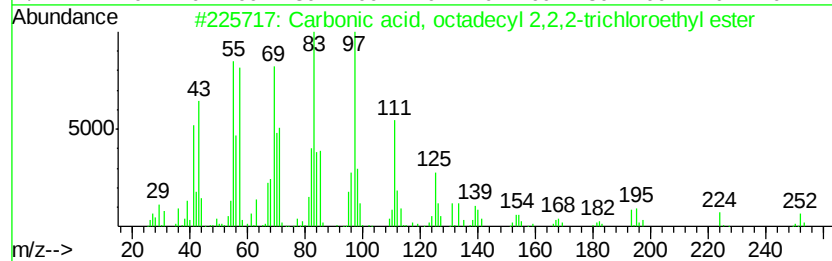
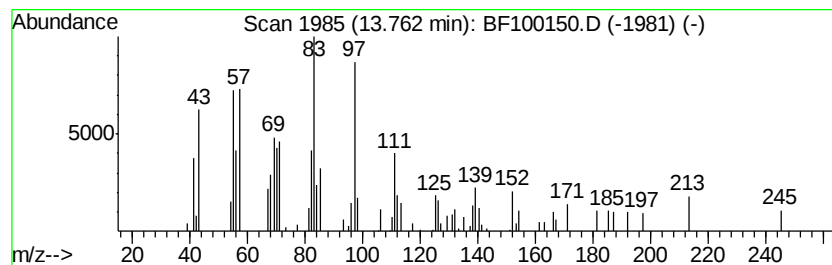
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Carbonic acid, octadecyl 2,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.22 ng	68050	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3		Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		1-Octadecene	252	C18H36	000112-88-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100150.D
Acq On : 3 Nov 2017 22:20
Operator : SJ/JU
Sample : I6294-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N48971

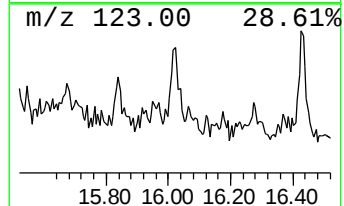
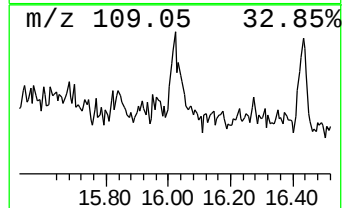
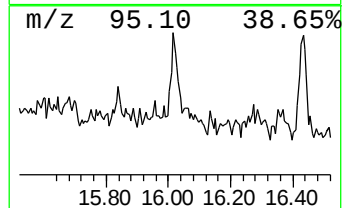
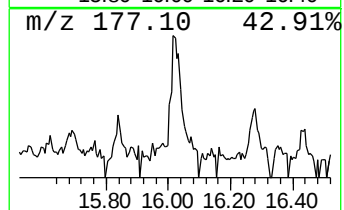
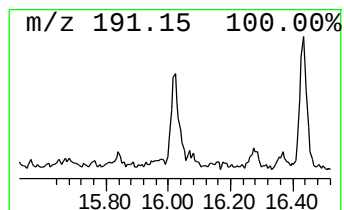
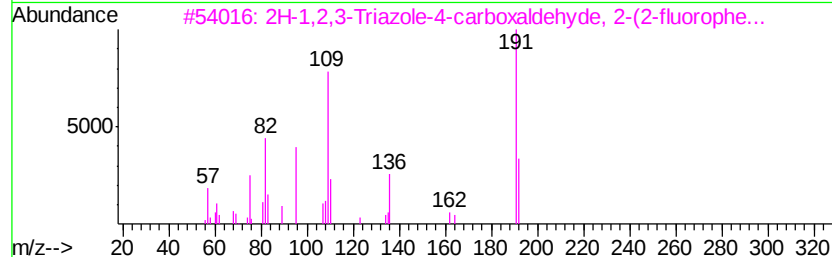
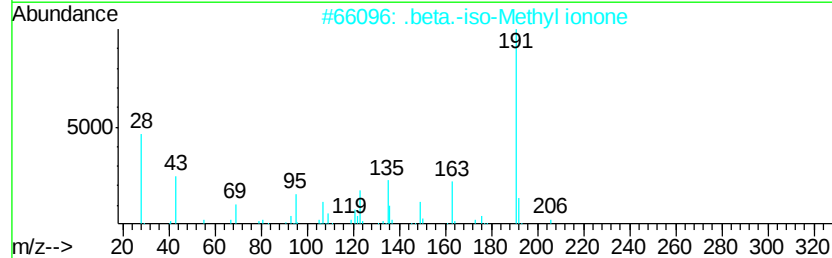
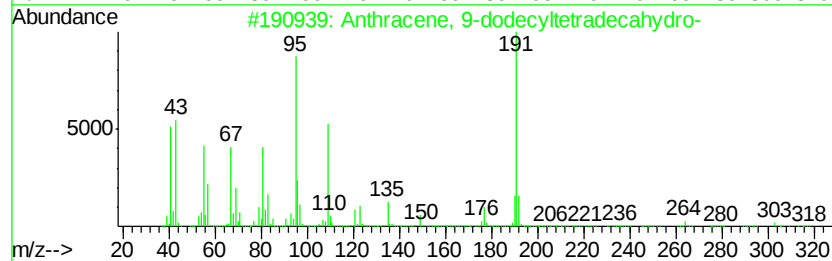
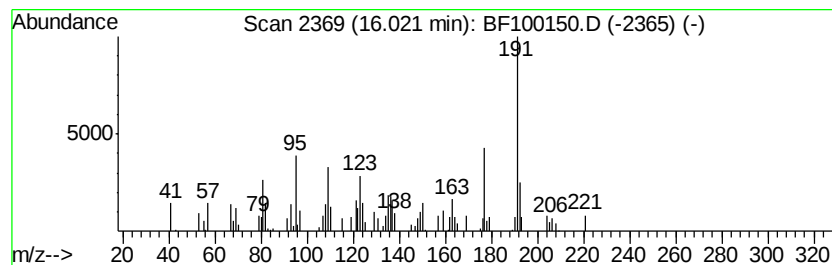
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.11 ng	88613	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	47
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
3		2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	38
4		2,5,5,8a-Tetramethyl-4-methylene...	206	C14H22O	093175-76-9	37
5		2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100150.D
Acq On : 3 Nov 2017 22:20
Operator : SJ/JU
Sample : I6294-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N48971

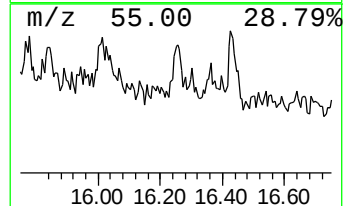
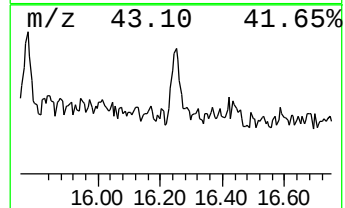
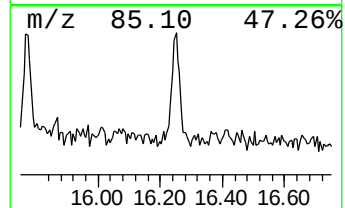
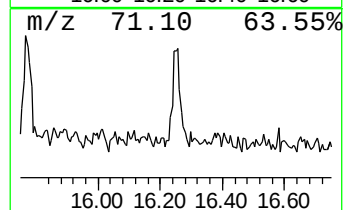
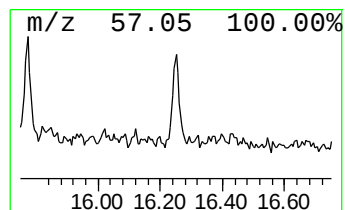
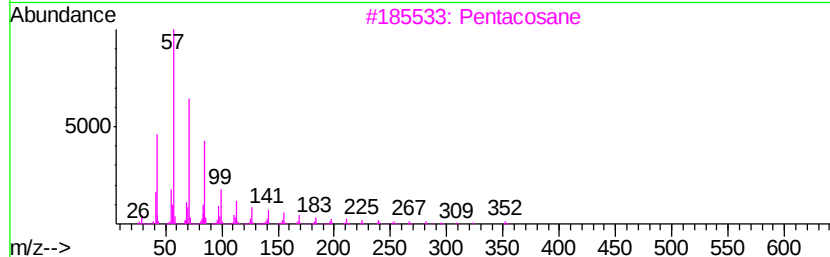
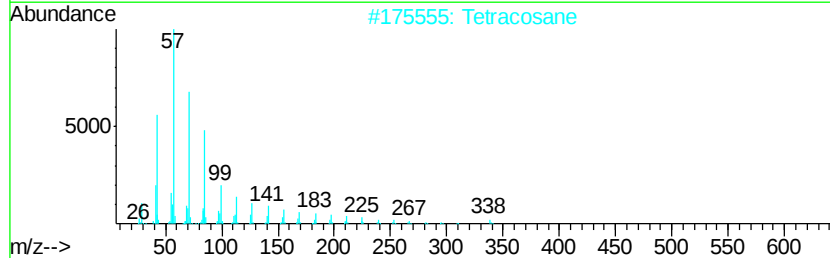
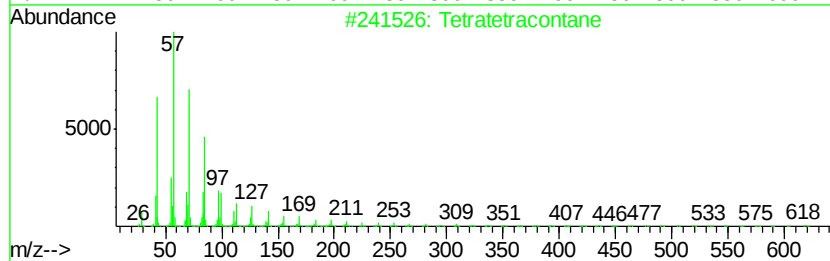
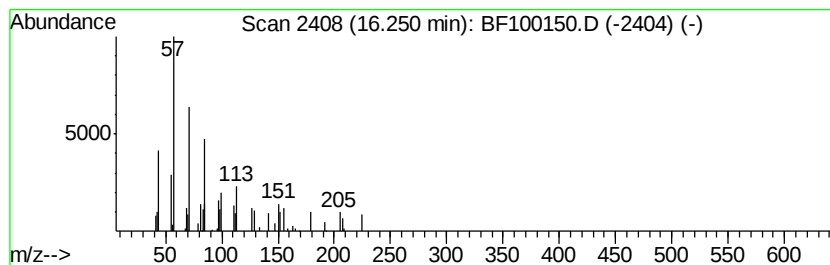
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	3.19 ng	68697	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	53
2		Tetracosane	338	C24H50	000646-31-1	53
3		Pentacosane	352	C25H52	000629-99-2	53
4		Octacosane	394	C28H58	000630-02-4	53
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100150.D
Acq On : 3 Nov 2017 22:20
Operator : SJ/JU
Sample : I6294-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
N48971

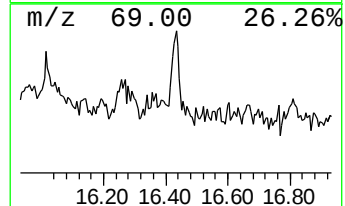
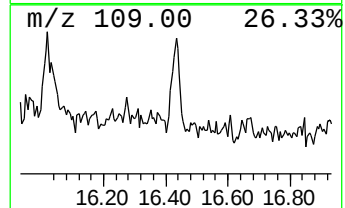
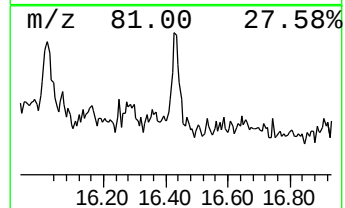
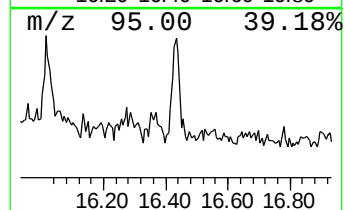
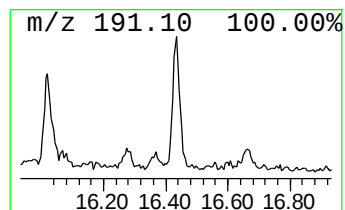
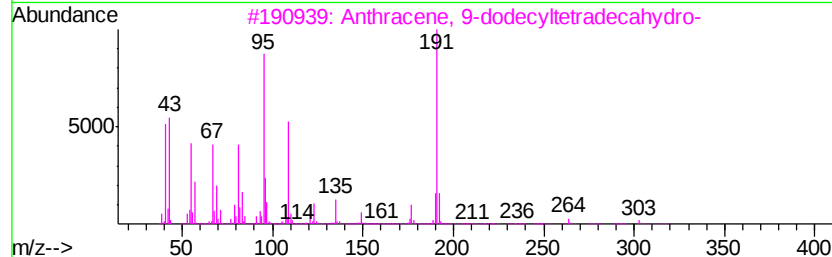
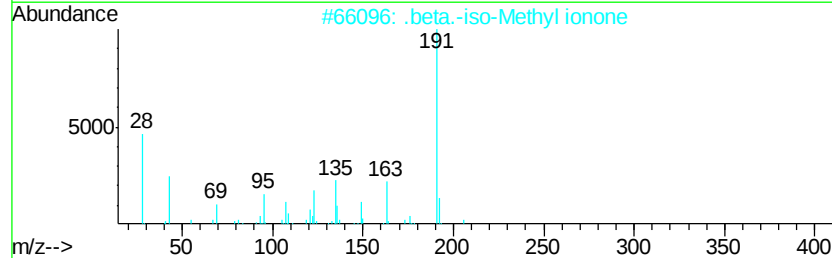
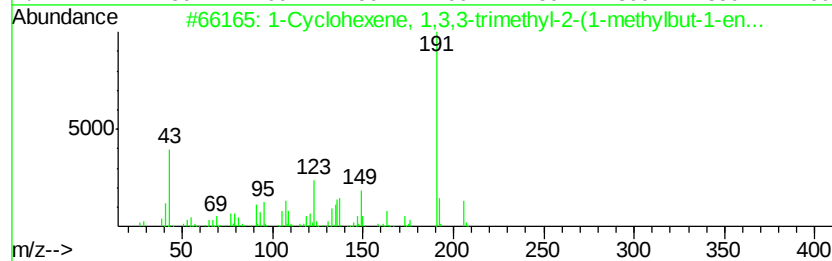
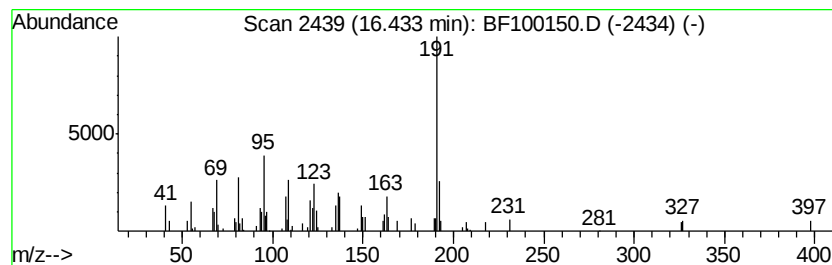
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Cyclohexene, 1,3,3-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	3.61 ng	77905	Perylene-d12	15.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	50
2			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	40
3			Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	40
4			2H-1,2,3-Triazole-4-carboxalde...	191	C9H6FN3O	051306-43-5	38
5			2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100150.D
Acq On : 3 Nov 2017 22:20
Operator : SJ/JU
Sample : I6294-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N48971

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	4.99	5.0 ng		129334	1	6.77	515551	20.0
unknown6.55	6.55	77.0 ng		1984160	1	6.77	515551	20.0
Phenol, p-tert-bu...	8.63	2.3 ng		83194	2	8.05	725679	20.0
n-Hexadecanoic acid	11.81	2.1 ng		72120	4	11.30	674123	20.0
Phenol, 4,4'-(1-m...	12.77	28.9 ng		610346	5	13.95	422131	20.0
Carbonic acid, oc...	13.76	3.2 ng		68050	5	13.95	422131	20.0
unknown16.02	16.02	4.1 ng		88613	6	15.41	431334	20.0
Tetratetracontane	16.25	3.2 ng		68697	6	15.41	431334	20.0
1-Cyclohexene, 1,...	16.43	3.6 ng		77905	6	15.41	431334	20.0