

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
 Data File : BF108973.D
 Acq On : 13 Sep 2018 19:16
 Operator : JU/SJ
 Sample : J4875-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091118-JETT-F-D-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	4.907	434	437	446	rBV	120105	133536	2.92%	0.452%
2	5.331	505	509	513	rBV	1499005	1318345	28.85%	4.459%
3	6.354	679	683	691	rBV	1174085	943121	20.64%	3.190%
4	6.495	702	707	710	rBV	2824000	2426036	53.09%	8.205%
5	6.725	743	746	750	rBV	1003821	868285	19.00%	2.937%
6	6.889	769	774	777	rBV	3184139	3115218	68.18%	10.536%
7	7.289	836	842	845	rBV	2749312	2737471	59.91%	9.258%
8	8.007	960	964	968	rBV	1267222	1062410	23.25%	3.593%
9	9.089	1143	1148	1151	rBV	4976490	4569418	100.00%	15.454%
10	9.478	1210	1214	1217	rBV	580669	456854	10.00%	1.545%
11	9.760	1258	1262	1265	rBV	1429086	1216473	26.62%	4.114%
12	10.436	1374	1377	1381	rVB	118826	101196	2.21%	0.342%
13	10.542	1391	1395	1398	rBV	2292148	1950419	42.68%	6.597%
14	11.236	1509	1513	1516	rBV	1444923	1128684	24.70%	3.817%
15	11.777	1601	1605	1616	rBV2	103063	126614	2.77%	0.428%
16	12.824	1778	1783	1786	rBV	4223231	4207185	92.07%	14.229%
17	13.742	1935	1939	1951	rBV5	30582	97341	2.13%	0.329%
18	13.860	1955	1959	1963	rBV	1059866	987106	21.60%	3.339%
19	14.354	2040	2043	2046	rBV	60409	49877	1.09%	0.169%
20	14.648	2089	2093	2099	rBV	93125	92496	2.02%	0.313%
21	14.718	2101	2105	2110	rVB	192036	180846	3.96%	0.612%
22	14.965	2143	2147	2154	rVB	112185	128381	2.81%	0.434%
23	15.265	2193	2198	2203	rBV	876232	1029149	22.52%	3.481%
24	15.324	2203	2208	2214	rVB	142899	181992	3.98%	0.616%
25	15.730	2272	2277	2284	rBV	148472	211911	4.64%	0.717%
26	16.201	2351	2357	2363	rBV2	101176	165569	3.62%	0.560%
27	16.748	2445	2450	2455	rBV2	39674	81305	1.78%	0.275%

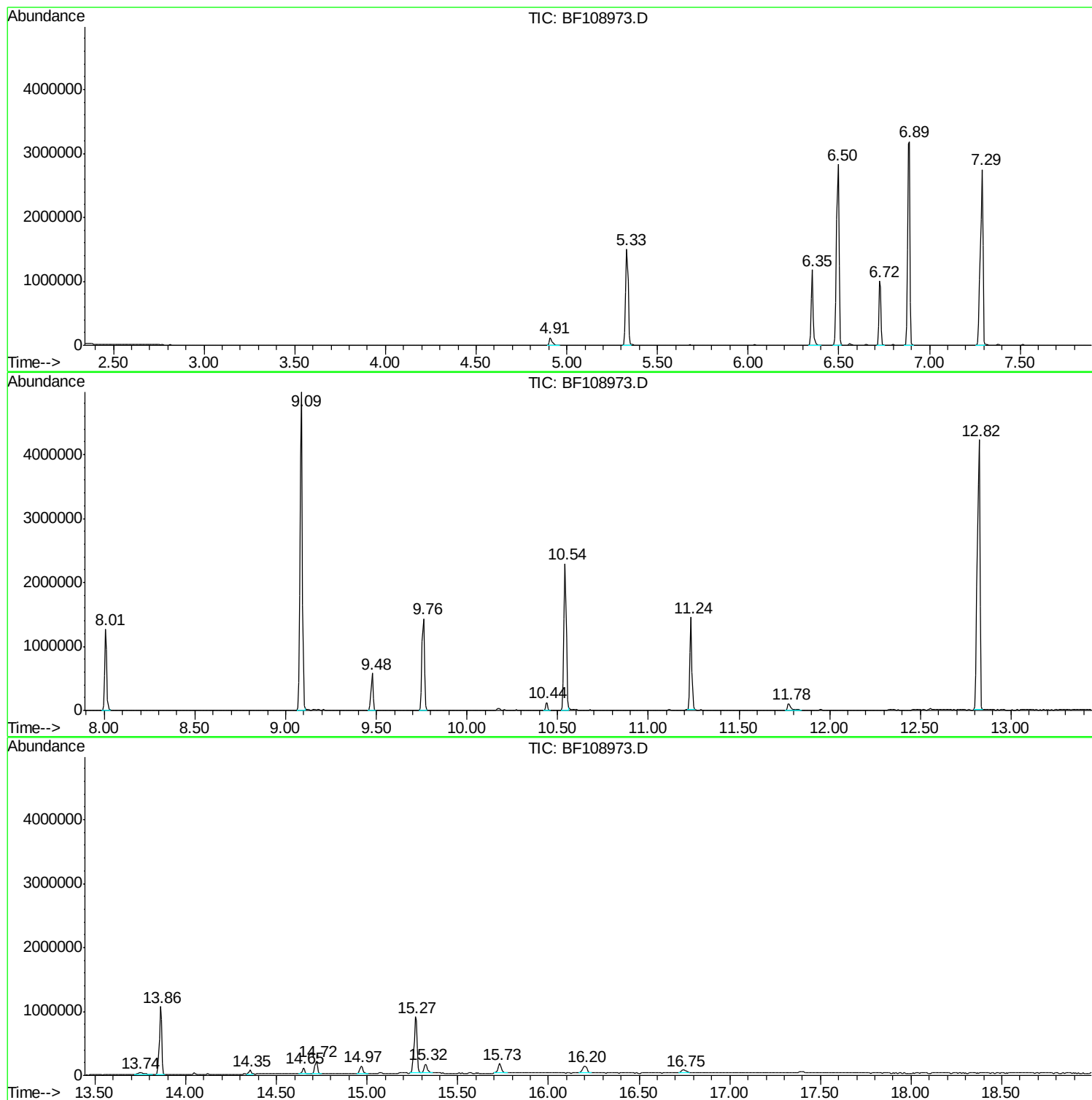
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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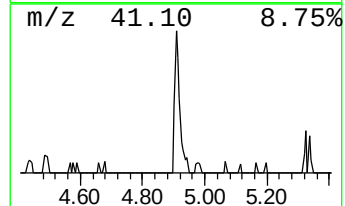
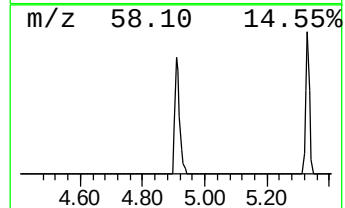
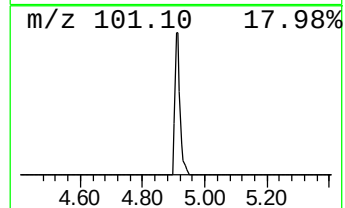
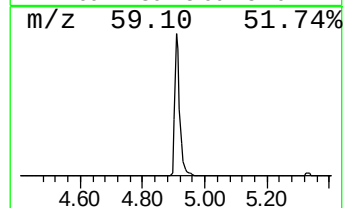
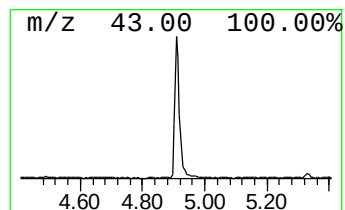
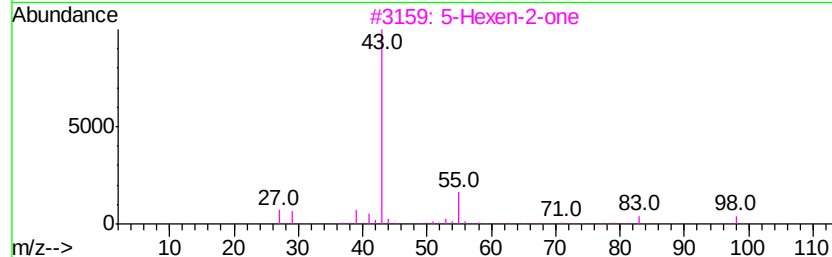
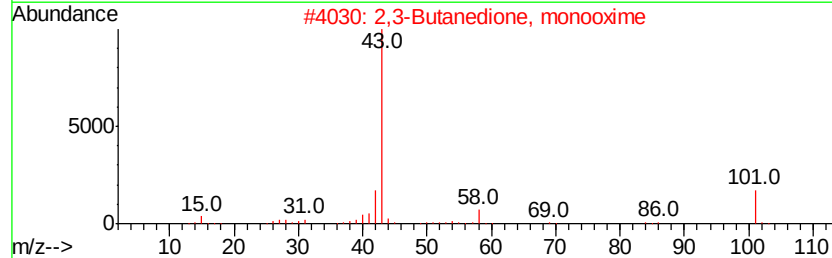
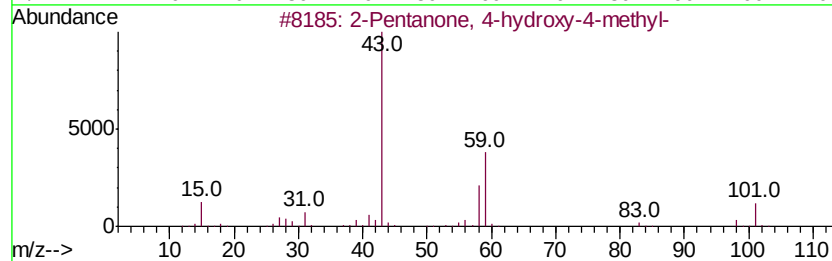
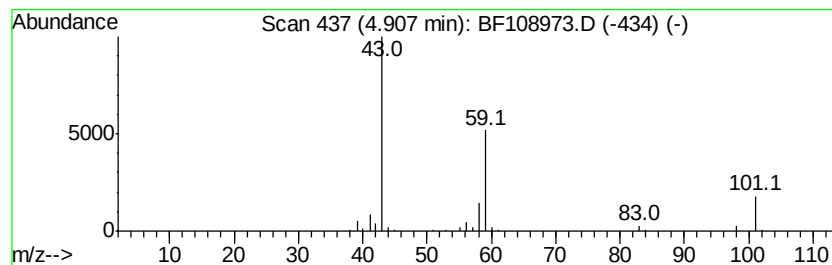
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.08 ng	133536	1,4-Dichlorobenzene-d4	6.72

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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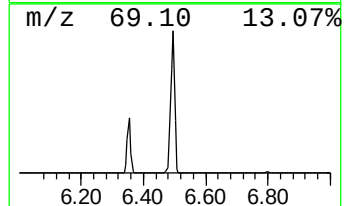
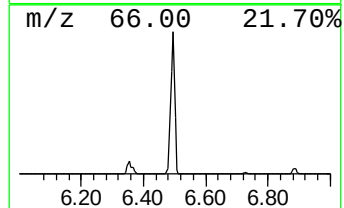
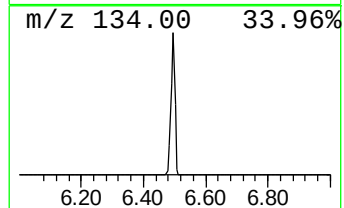
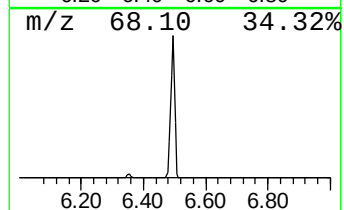
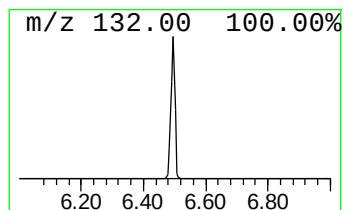
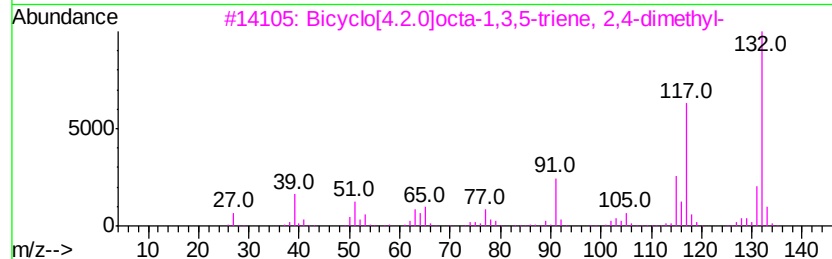
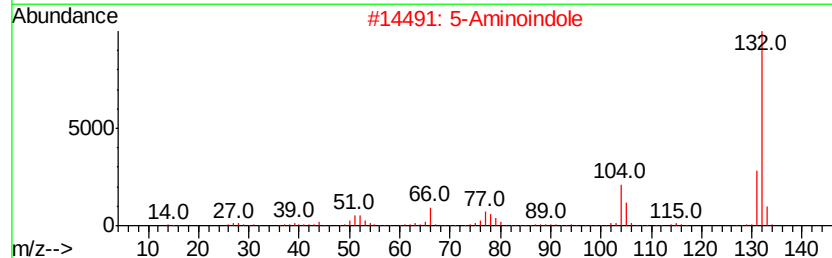
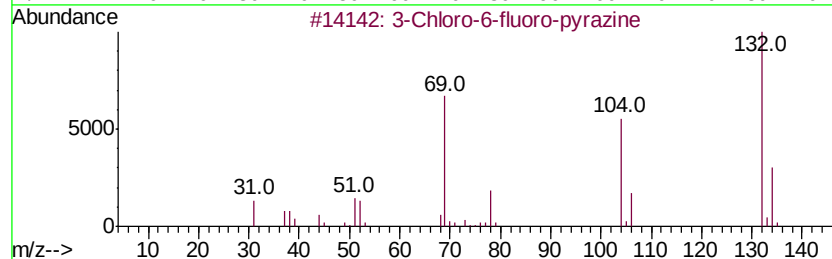
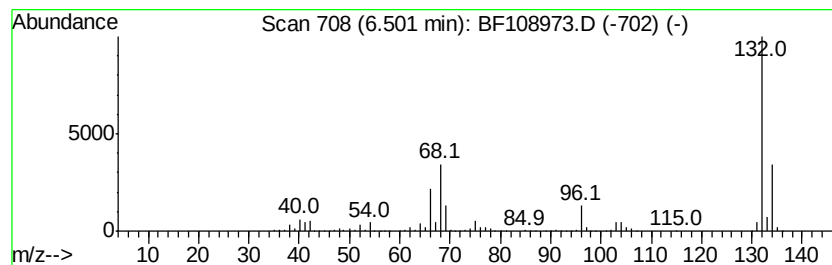
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Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	55.88 ng	2426040	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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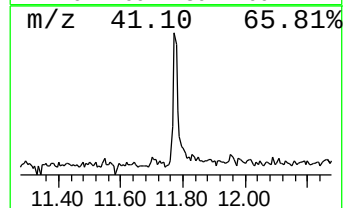
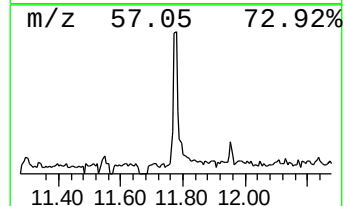
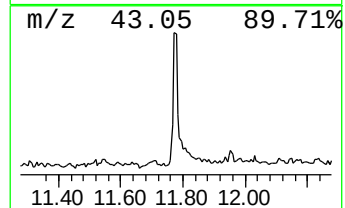
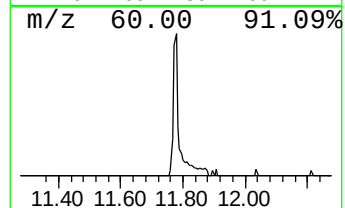
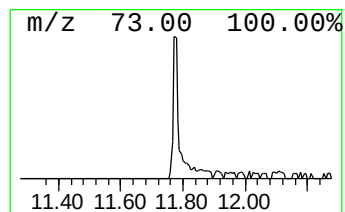
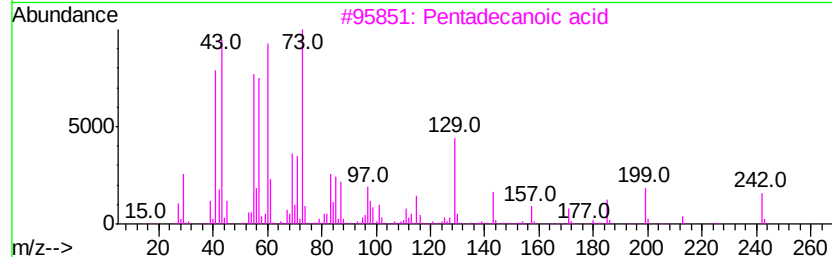
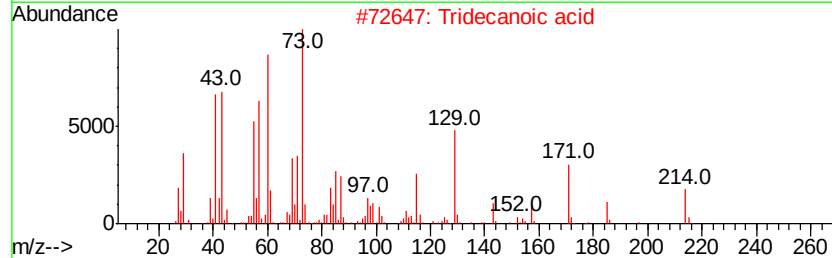
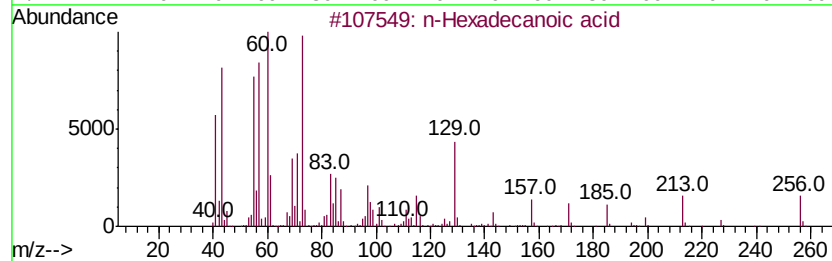
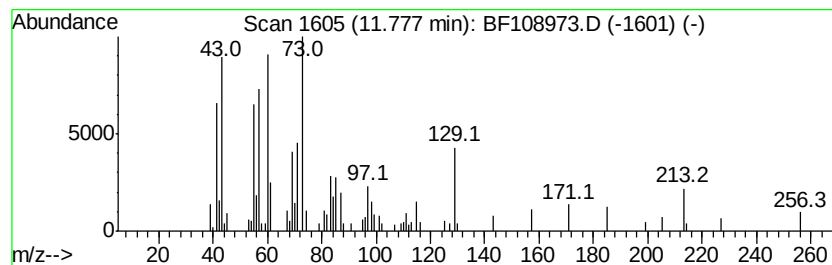
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.24 ng	126614	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18



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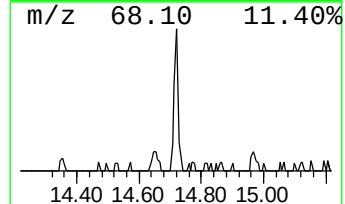
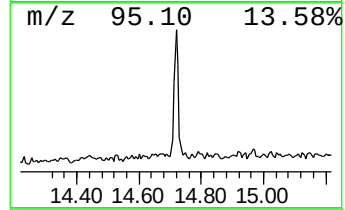
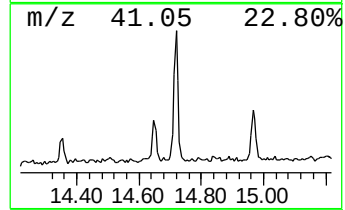
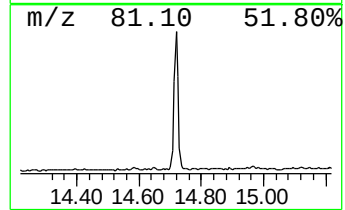
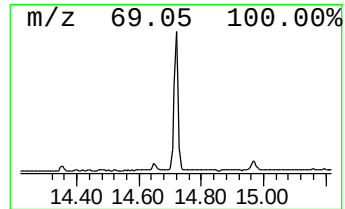
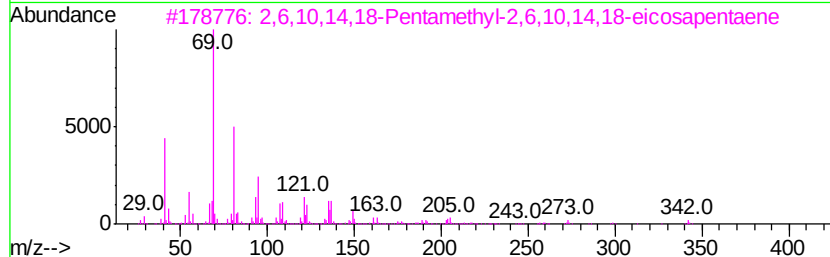
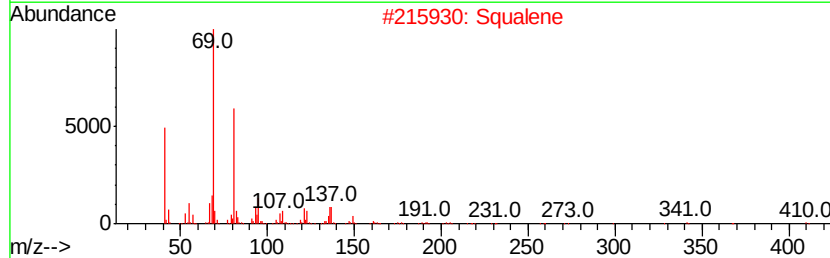
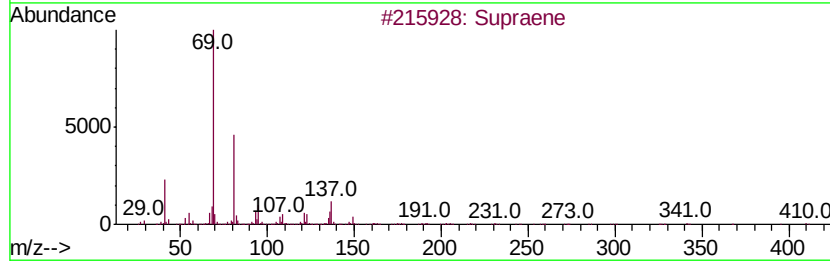
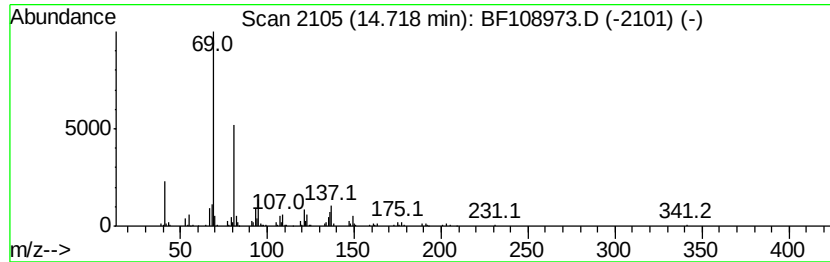
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.51 ng	180846	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	91
3	2,6,10,14,18-Pentamethyl-2,6,10,...		342	C25H42	075581-03-2	83
4	2,6,10,14-Hexadecatetraenoic aci...		332	C22H36O2	024035-35-6	72
5	1,6-Octadiene, 3,5-dimethyl-, tr...		138	C10H18	074630-87-8	50



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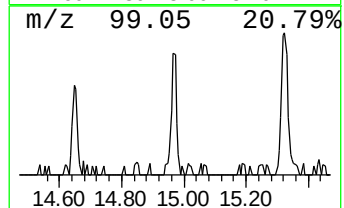
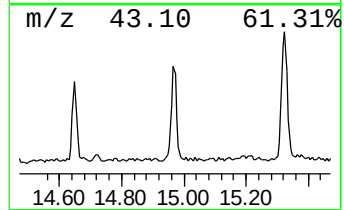
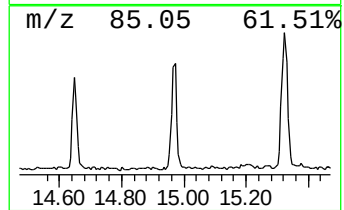
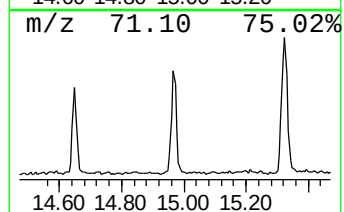
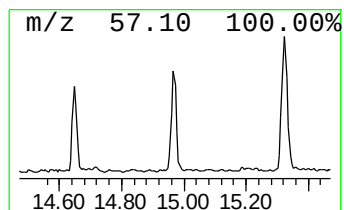
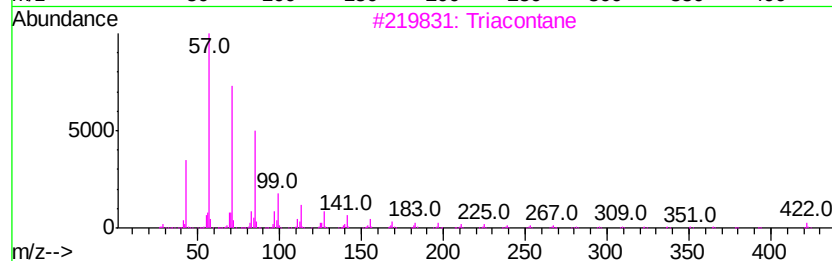
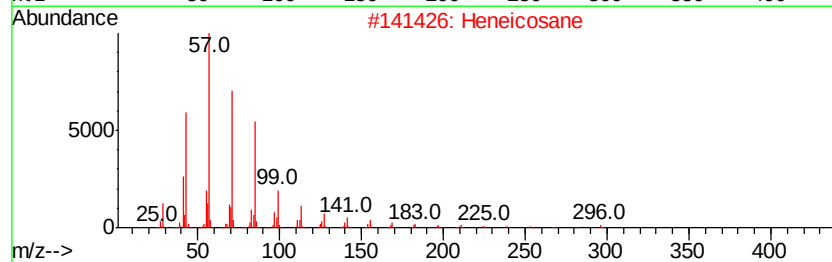
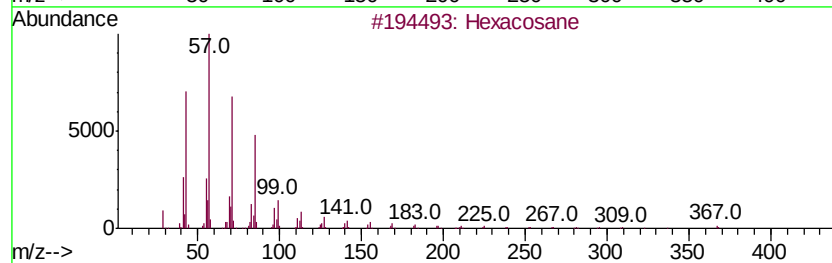
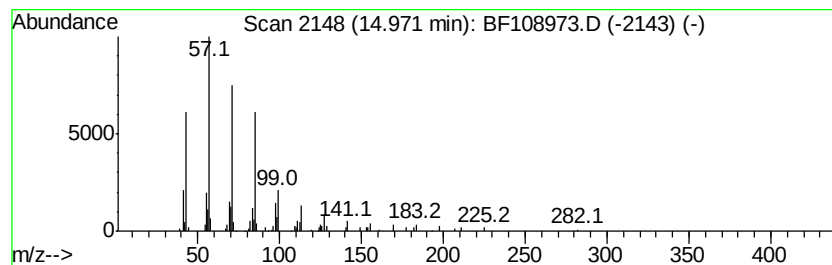
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Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.49 ng	128381	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Hexadecane	226	C16H34	000544-76-3	91



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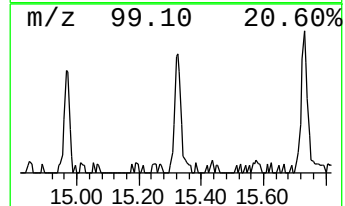
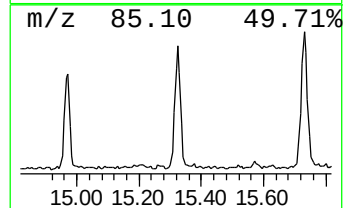
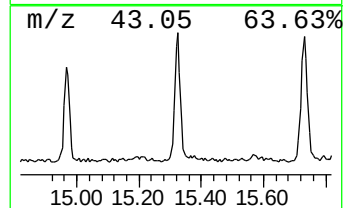
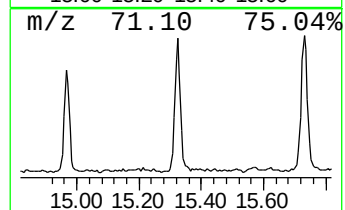
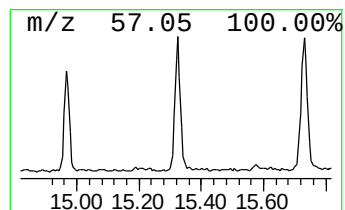
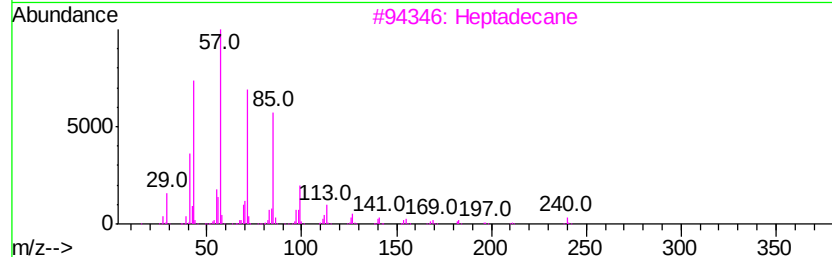
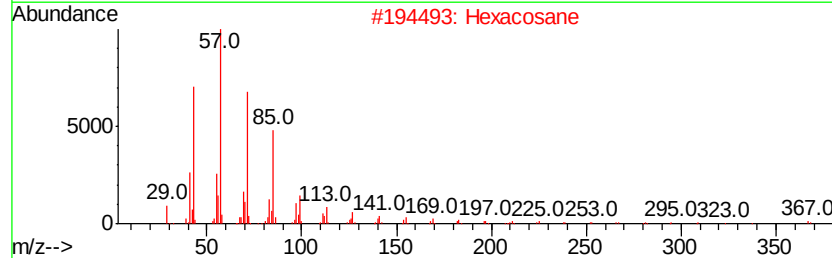
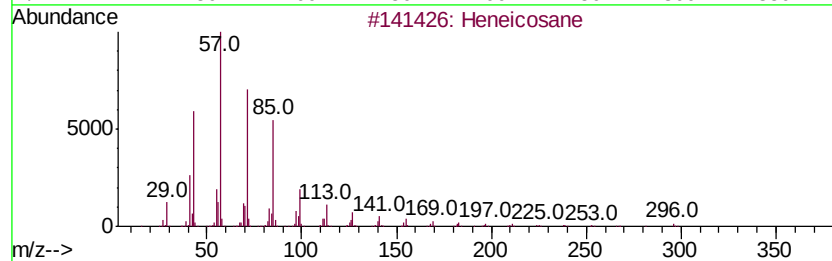
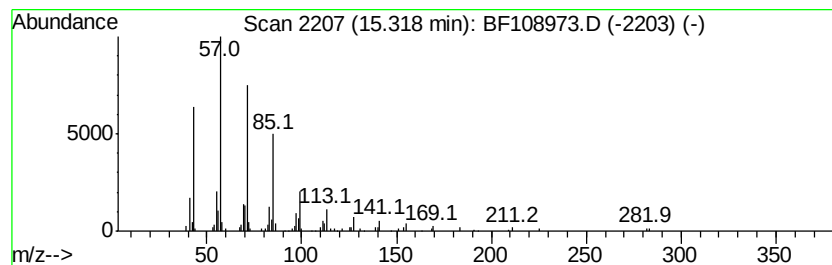
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	3.54 ng	181992	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heptadecane		240	C17H36	000629-78-7	91
4	Hexadecane		226	C16H34	000544-76-3	91
5	Tetracosane		338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108973.D
Acq On : 13 Sep 2018 19:16
Operator : JU/SJ
Sample : J4875-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-JETT-F-D-B

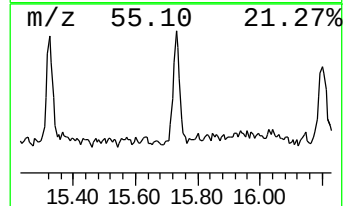
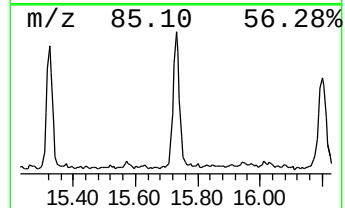
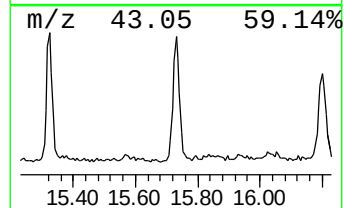
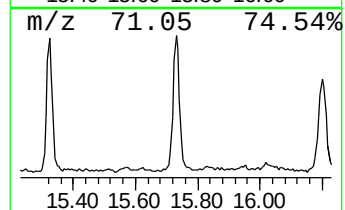
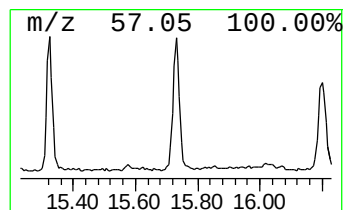
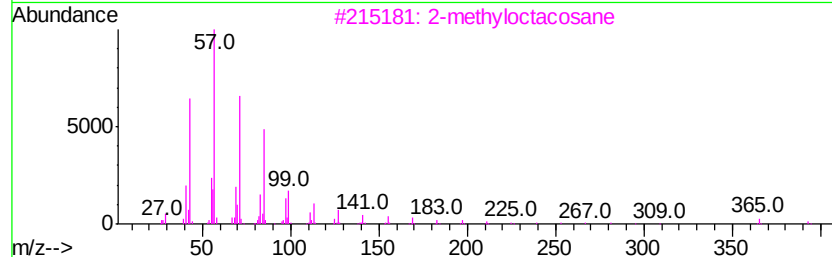
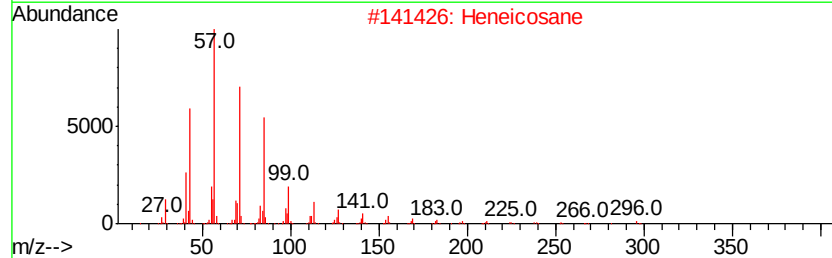
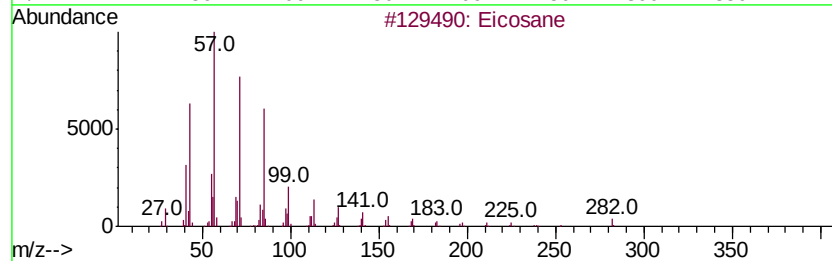
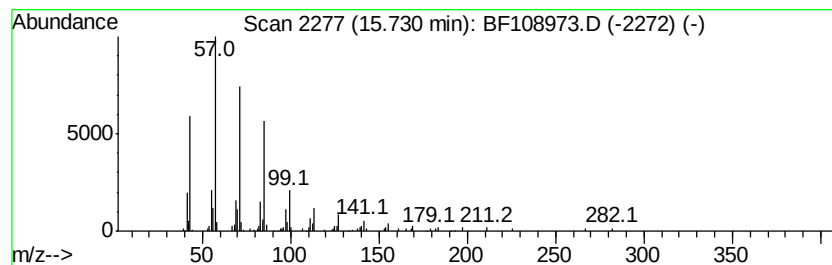
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	4.12 ng	211911	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	97
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108973.D
Acq On : 13 Sep 2018 19:16
Operator : JU/SJ
Sample : J4875-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-JETT-F-D-B

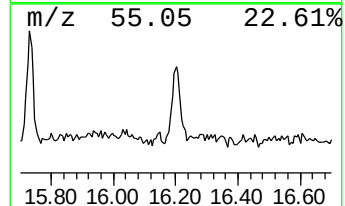
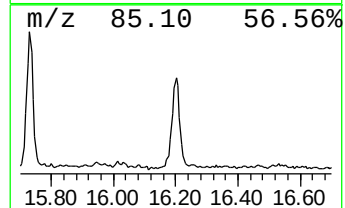
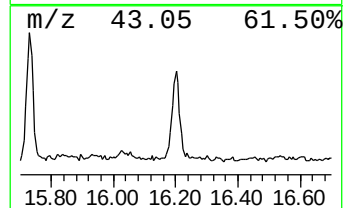
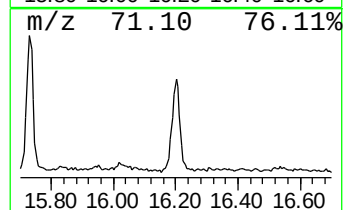
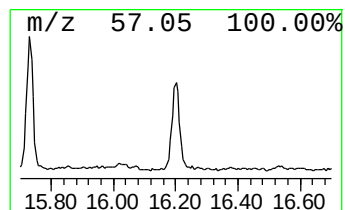
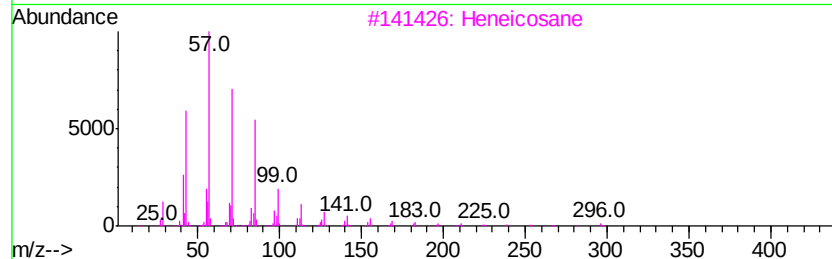
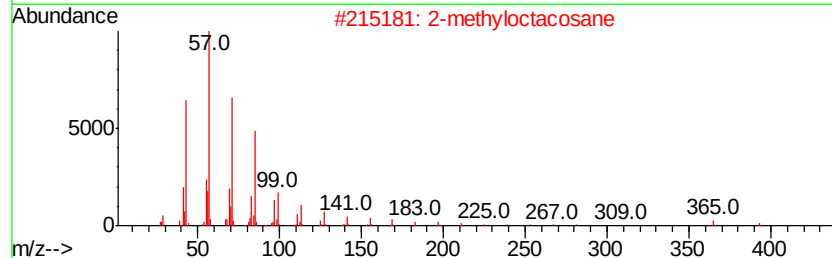
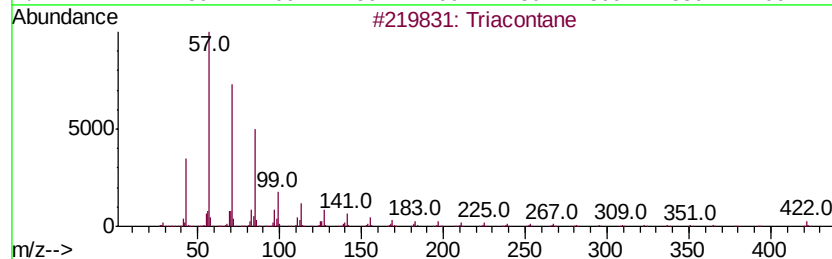
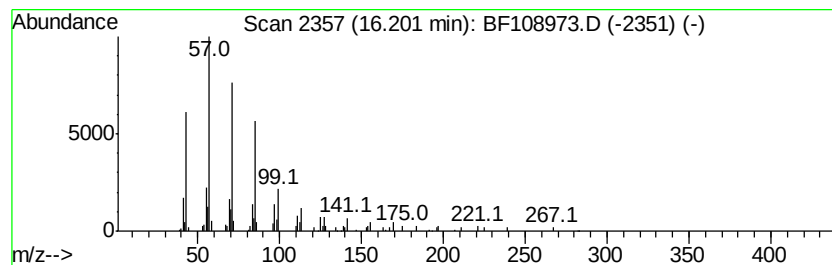
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.22 ng	165569	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
Data File : BF108973.D
Acq On : 13 Sep 2018 19:16
Operator : JU/SJ
Sample : J4875-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-JETT-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.91	3.1 ng		133536	1	6.72	868285	20.0
unknown6.50	6.50	55.9 ng		2426040	1	6.72	868285	20.0
n-Hexadecanoic acid	11.78	2.2 ng		126614	4	11.24	1128680	20.0
Supraene	14.72	3.5 ng		180846	6	15.27	1029150	20.0
Hexacosane	14.97	2.5 ng		128381	6	15.27	1029150	20.0
Heneicosane	15.32	3.5 ng		181992	6	15.27	1029150	20.0
Eicosane	15.73	4.1 ng		211911	6	15.27	1029150	20.0
Triacontane	16.20	3.2 ng		165569	6	15.27	1029150	20.0