

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072318\
 Data File : BF107598.D
 Acq On : 23 Jul 2018 19:46
 Operator : JU/SJ
 Sample : J4106-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MOLA-BOULEVARD

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-BF072018.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	5.219	486	490	506	rBV	805407	1035632	17.04%	1.944%
2	5.613	553	557	589	rBV	4882166	6079124	100.00%	11.409%
3	6.613	722	727	746	rBV	4670051	5960895	98.06%	11.187%
4	6.754	746	751	773	rVB	5383896	6050299	99.53%	11.354%
5	6.978	785	789	804	rBV	1430189	1521764	25.03%	2.856%
6	7.131	811	815	833	rBV	4306763	4725599	77.73%	8.868%
7	7.542	880	885	906	rBV	3148784	3723340	61.25%	6.988%
8	8.260	1003	1007	1034	rBV	1738516	1825323	30.03%	3.426%
9	9.336	1184	1190	1205	rBV	5891319	5755635	94.68%	10.801%
10	9.725	1252	1256	1262	rBV	330204	299541	4.93%	0.562%
11	10.019	1302	1306	1317	rBV2	1647774	1651341	27.16%	3.099%
12	10.813	1437	1441	1454	rBV	2912189	3350285	55.11%	6.287%
13	11.519	1557	1561	1569	rBV	1492606	1634863	26.89%	3.068%
14	12.019	1643	1646	1649	rBV2	97150	93090	1.53%	0.175%
15	12.060	1649	1653	1657	rVB	51852	72032	1.18%	0.135%
16	12.736	1764	1768	1771	rBV	75279	76086	1.25%	0.143%
17	12.954	1802	1805	1806	rBV2	97754	89246	1.47%	0.167%
18	13.101	1826	1830	1841	rBV	4974186	5085013	83.65%	9.543%
19	13.313	1863	1866	1869	rVB	114010	108031	1.78%	0.203%
20	13.566	1905	1909	1912	rBV6	43629	69147	1.14%	0.130%
21	13.654	1920	1924	1926	rBV2	201195	188524	3.10%	0.354%
22	13.983	1977	1980	1986	rBV	367062	321138	5.28%	0.603%
23	14.165	2007	2011	2019	rBV	1439346	1565205	25.75%	2.937%
24	14.301	2031	2034	2038	rBV	263295	256311	4.22%	0.481%
25	14.607	2083	2086	2090	rBV	289444	273566	4.50%	0.513%
26	14.930	2138	2141	2144	rVB	201657	196234	3.23%	0.368%
27	15.289	2199	2202	2205	rVB	163630	173115	2.85%	0.325%
28	15.707	2268	2273	2280	rVB	736595	1105259	18.18%	2.074%

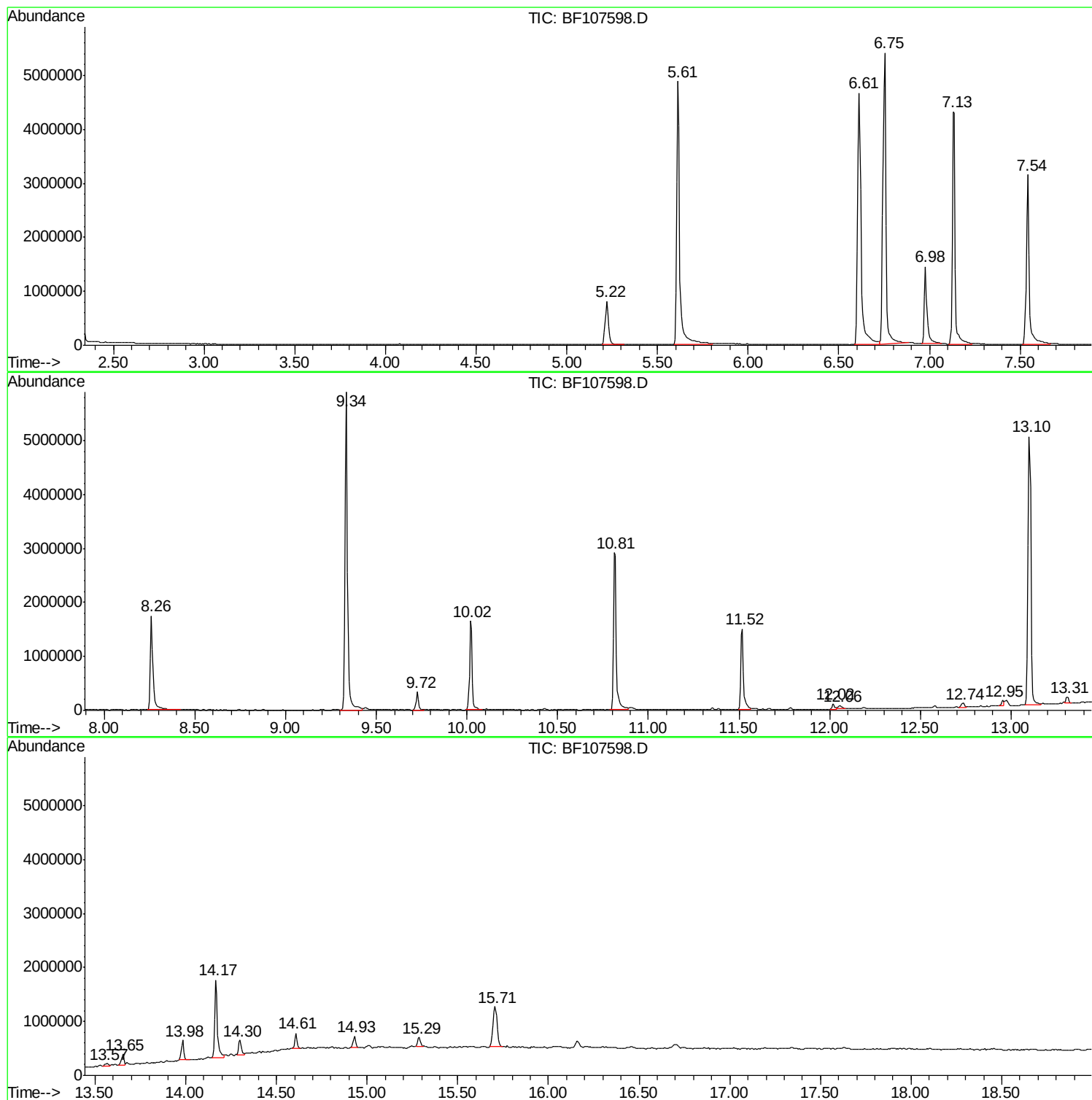
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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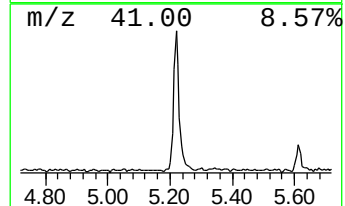
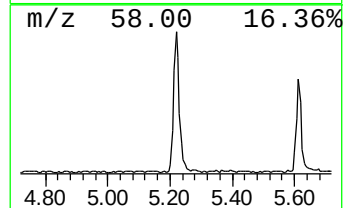
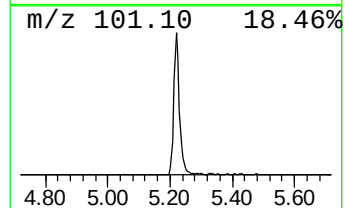
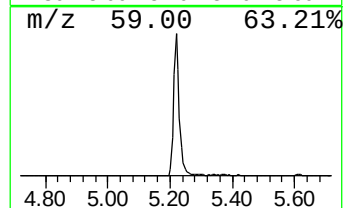
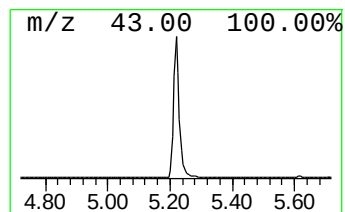
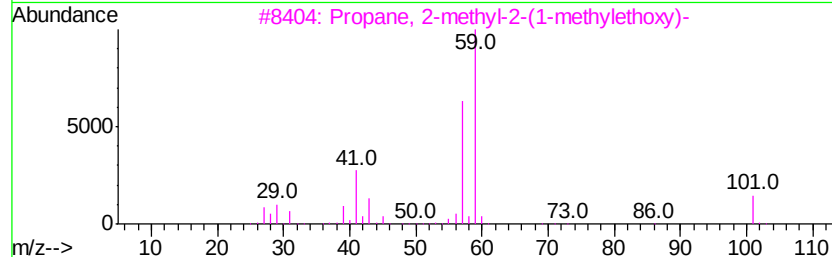
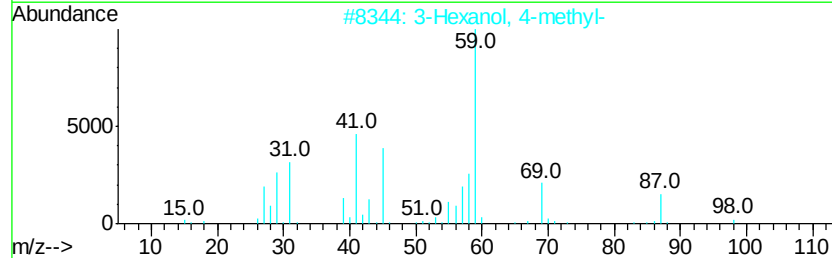
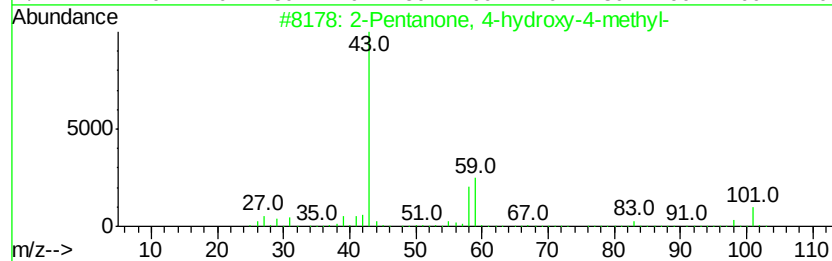
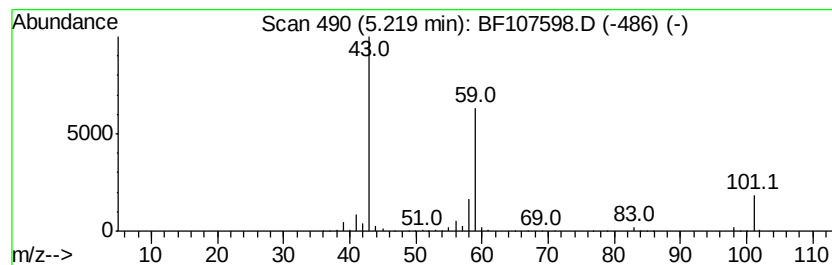
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.22	13.61 ng	1035630	1,4-Dichlorobenzene-d4	6.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
5			Guanidine	59	CH5N3	000113-00-8	9



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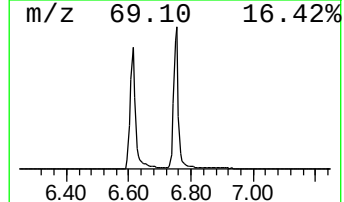
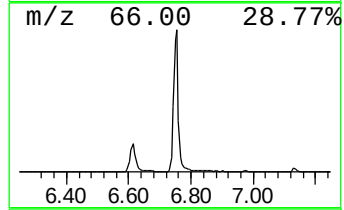
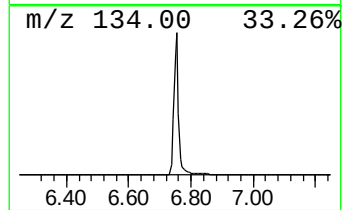
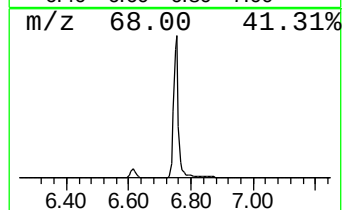
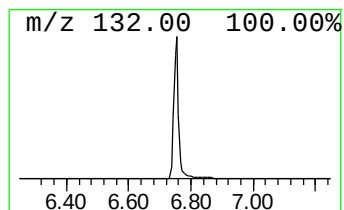
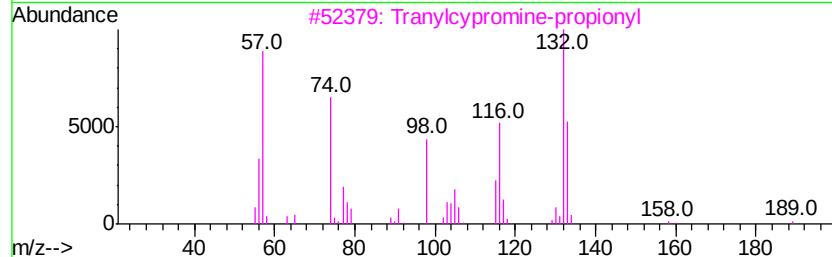
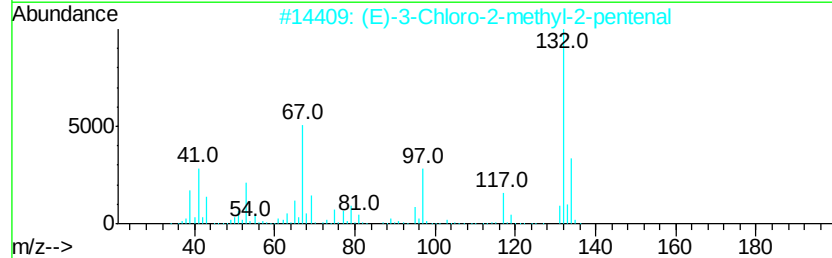
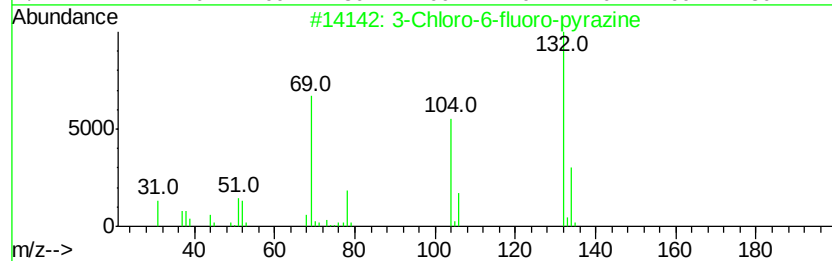
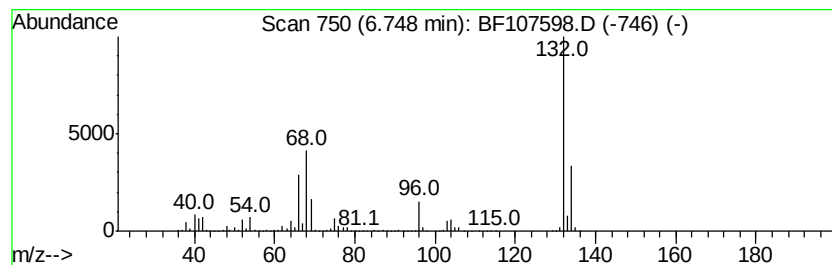
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	79.52 ng	6050300	1,4-Dichlorobenzene-d4	6.98

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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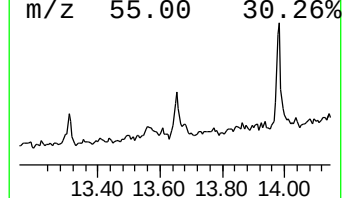
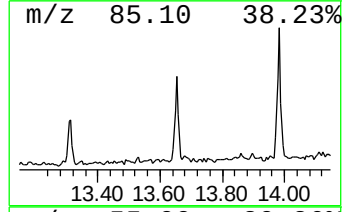
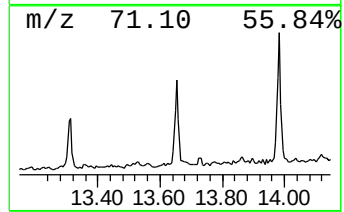
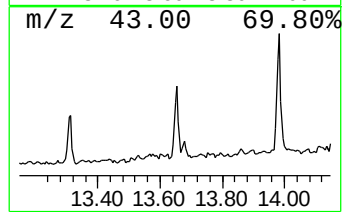
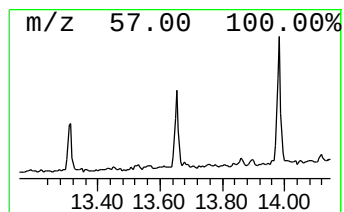
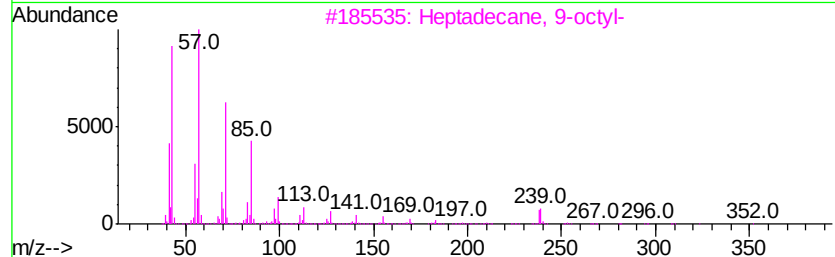
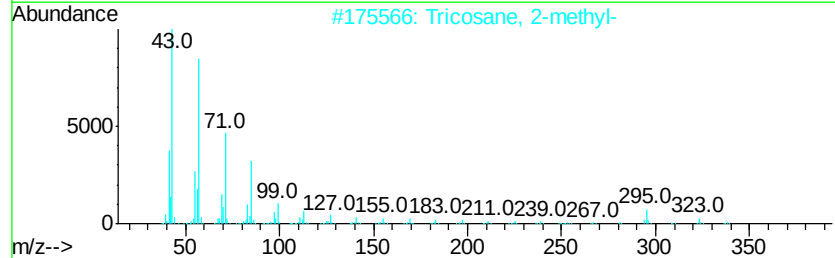
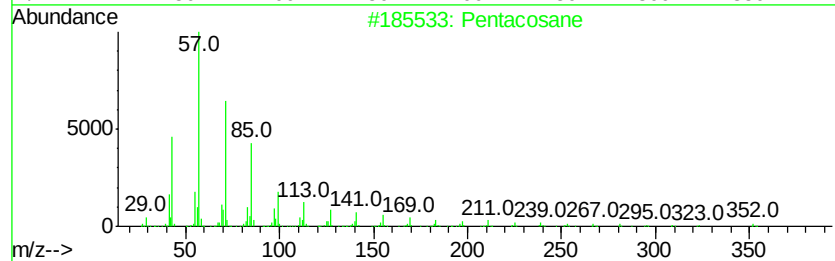
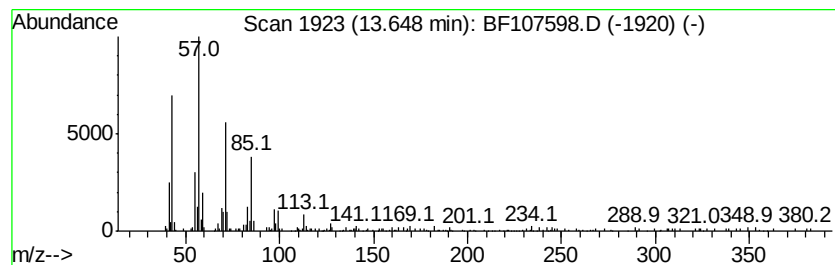
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Peak Number 4 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	2.41 ng	188524	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	93
2	Tricosane, 2-methyl-		338	C24H50	001928-30-9	90
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
4	Heptacosane		380	C27H56	000593-49-7	86
5	Heneicosane		296	C21H44	000629-94-7	81



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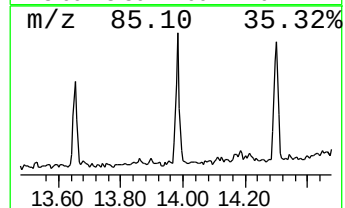
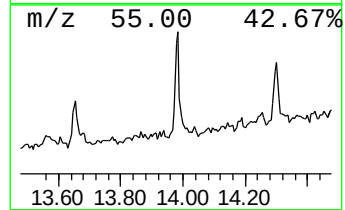
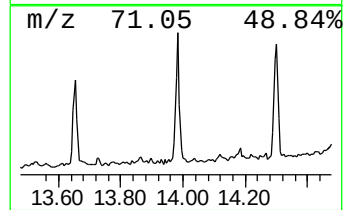
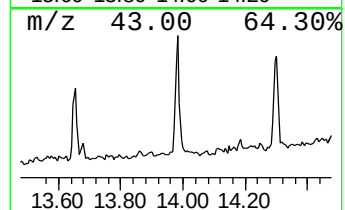
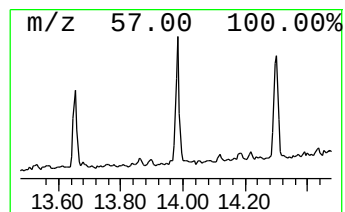
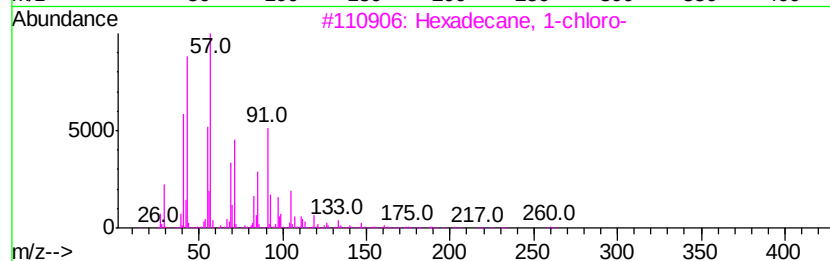
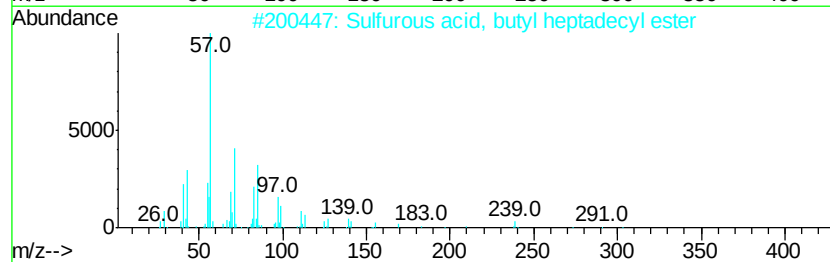
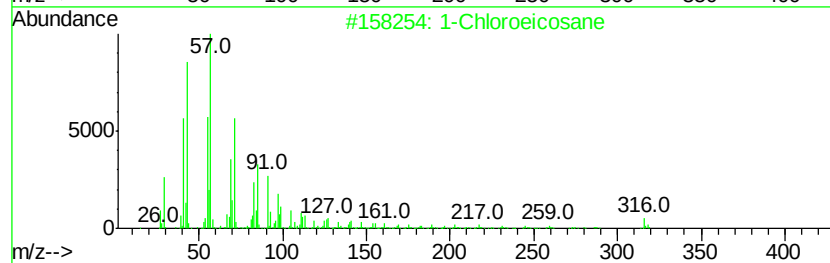
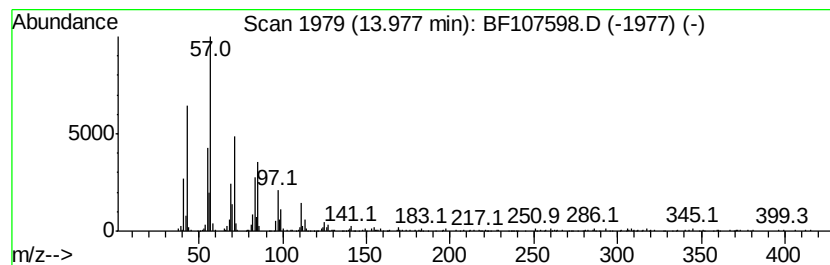
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Peak Number 5 1-Chloroeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	4.10 ng	321138	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Chloroeicosane	316	C20H41Cl	042217-02-7	94
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
3		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	91
4		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	91
5		Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	91



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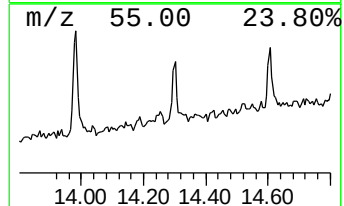
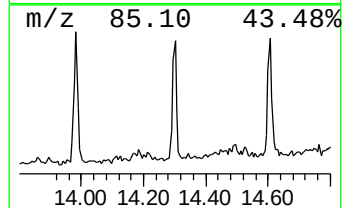
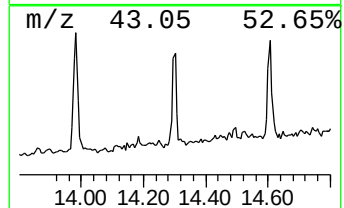
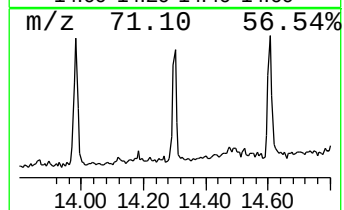
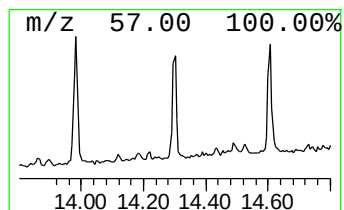
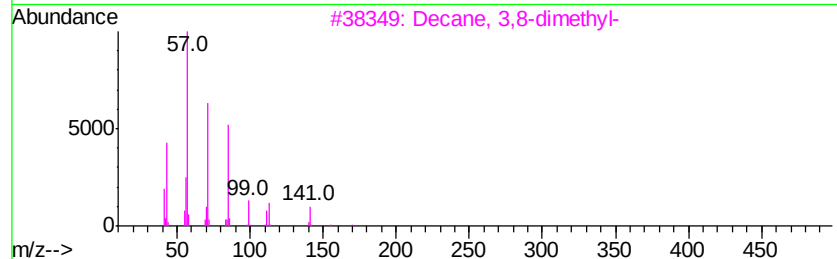
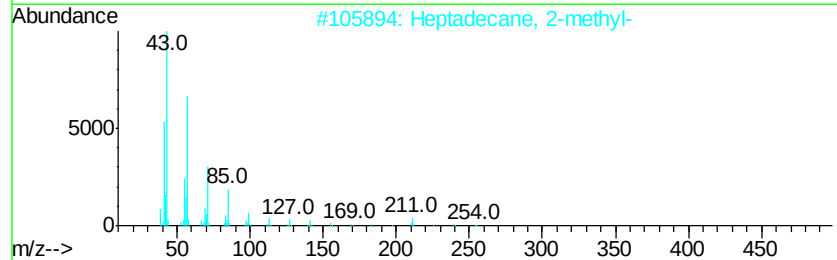
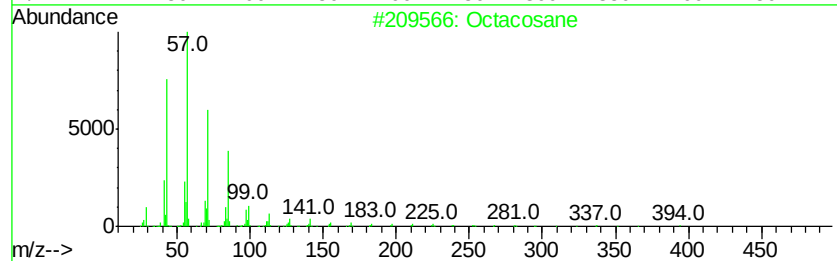
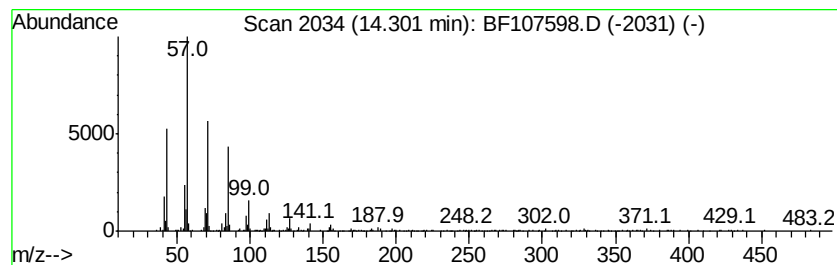
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	3.28 ng	256311	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	94
2	Heptadecane, 2-methyl-		254	C18H38	001560-89-0	90
3	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	90
4	Heneicosane		296	C21H44	000629-94-7	86
5	Eicosane		282	C20H42	000112-95-8	86



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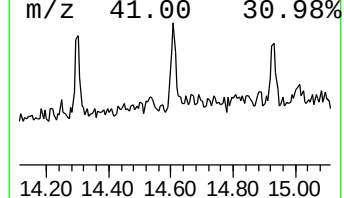
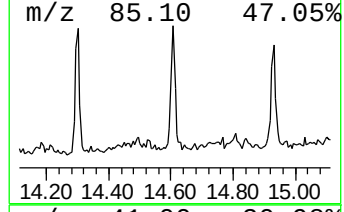
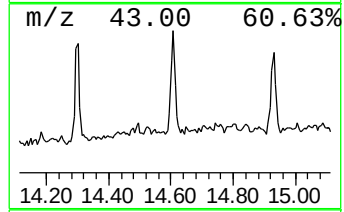
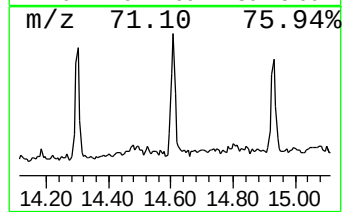
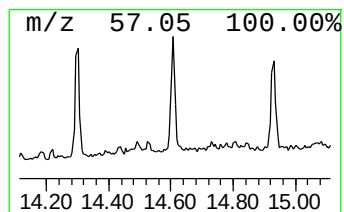
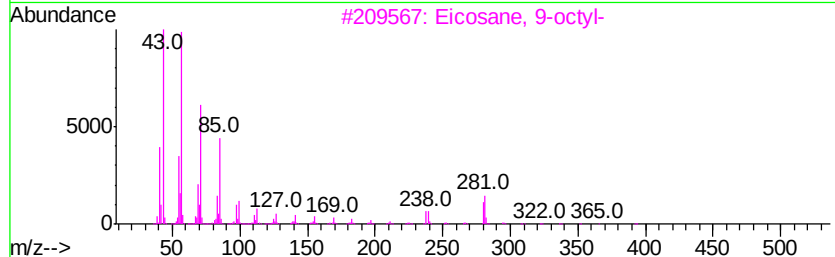
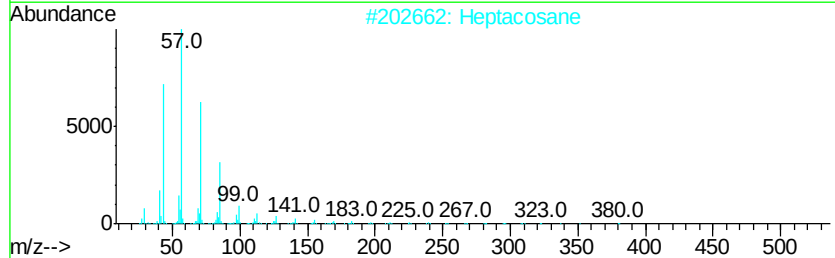
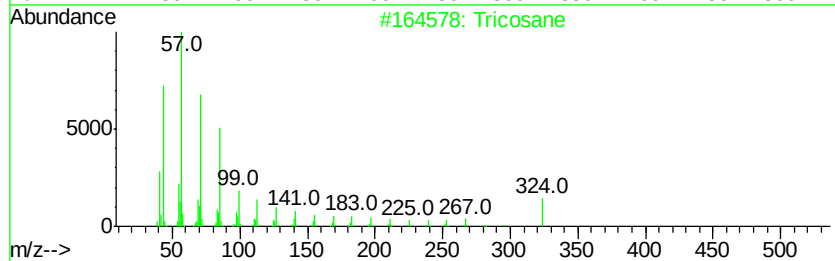
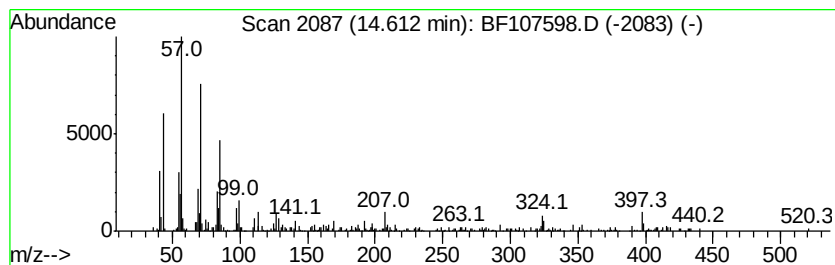
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	3.50 ng	273566	Chrysene-d12	14.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	91
2	Heptacosane		380	C27H56	000593-49-7	87
3	Eicosane, 9-octyl-		394	C28H58	013475-77-9	87
4	Tetracosane		338	C24H50	000646-31-1	83
5	Behenyl chloride		344	C22H45Cl	042217-03-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107598.D
Acq On : 23 Jul 2018 19:46
Operator : JU/SJ
Sample : J4106-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOLA-BOULEVARD

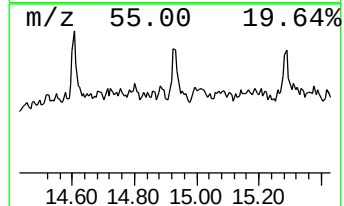
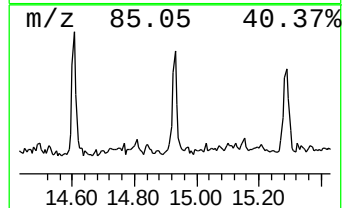
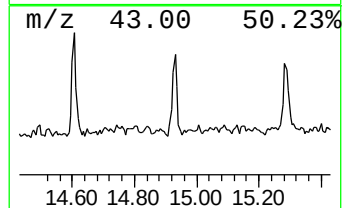
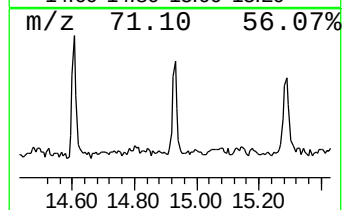
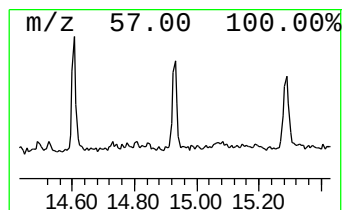
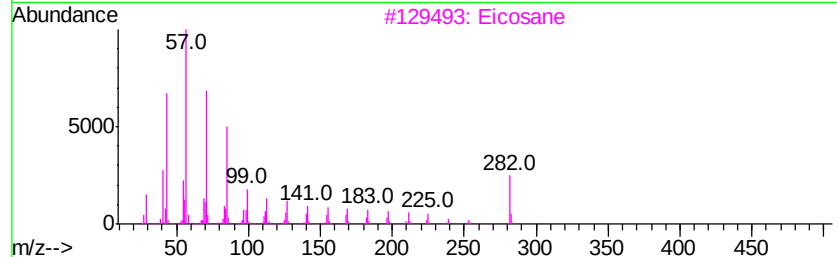
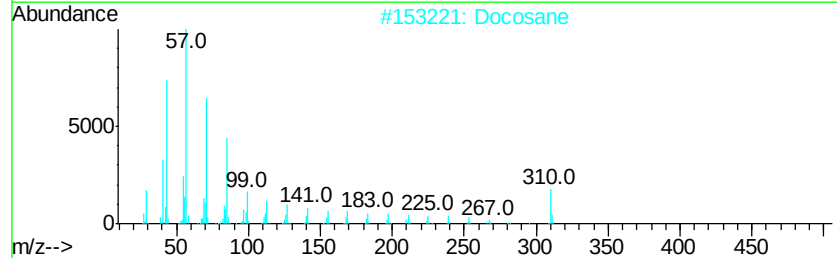
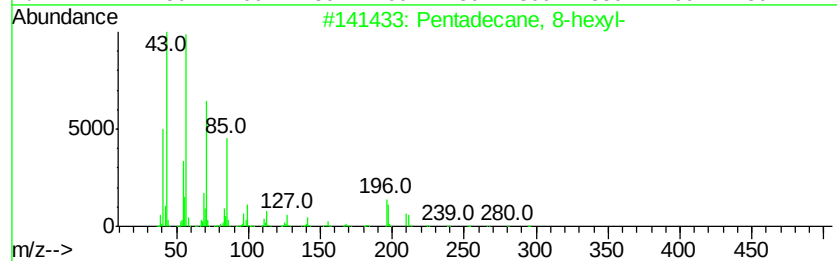
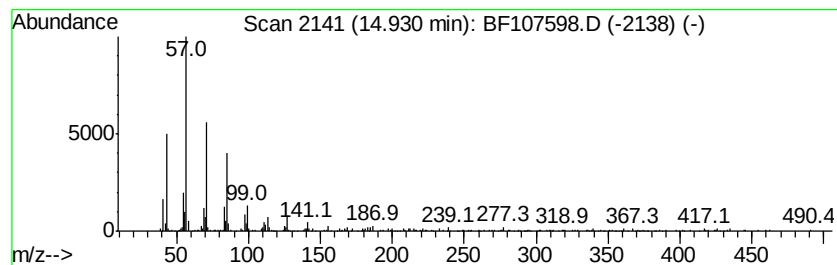
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.51 ng	196234	Chrysene-d12	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
2		Docosane	310	C22H46	000629-97-0	83
3		Eicosane	282	C20H42	000112-95-8	83
4		Heptacosane	380	C27H56	000593-49-7	83
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107598.D
Acq On : 23 Jul 2018 19:46
Operator : JU/SJ
Sample : J4106-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOLA-BOULEVARD

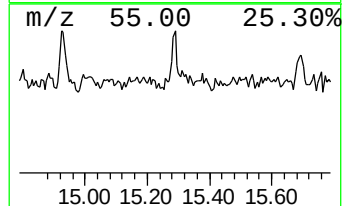
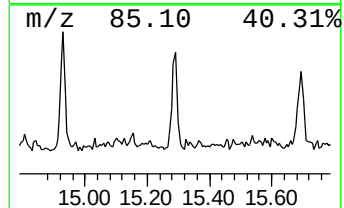
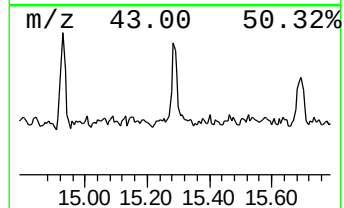
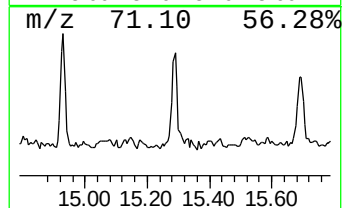
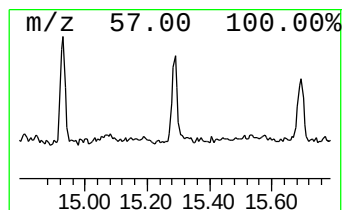
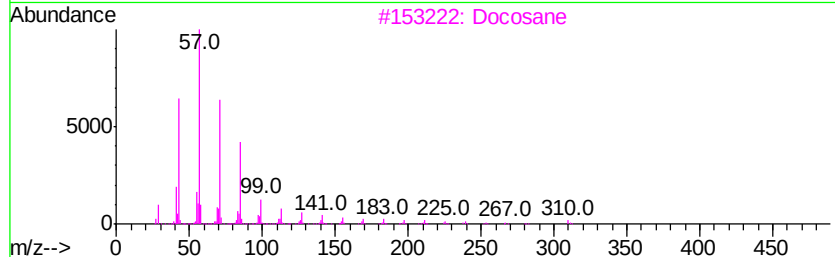
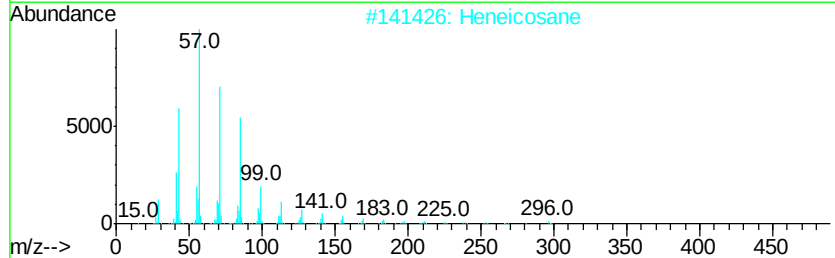
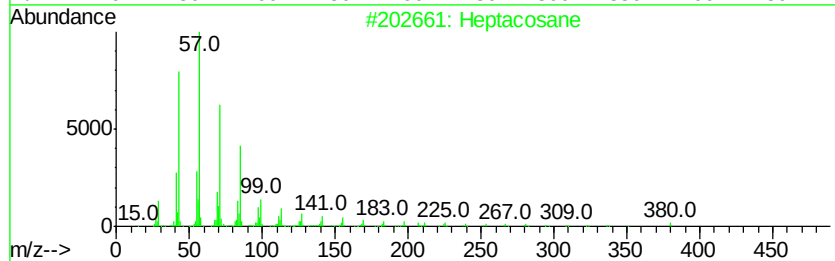
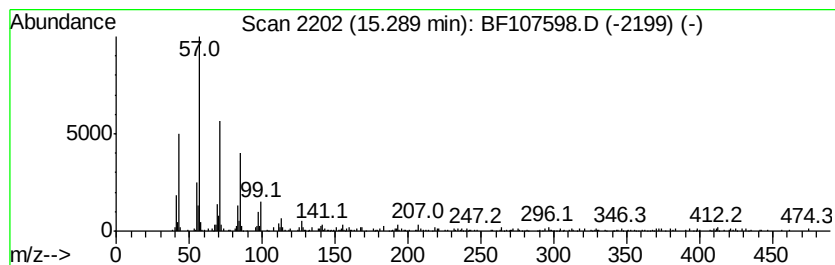
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	3.13 ng	173115	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	95
2		Heneicosane	296	C21H44	000629-94-7	90
3		Docosane	310	C22H46	000629-97-0	81
4		Heptadecane	240	C17H36	000629-78-7	74
5		2-methyloctacosane	408	C29H60	1000376-72-8	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072318\
Data File : BF107598.D
Acq On : 23 Jul 2018 19:46
Operator : JU/SJ
Sample : J4106-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOLA-BOULEVARD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.22	13.6	ng	1035630	1	6.98	1521760	20.0
unknown6.75	6.75	79.5	ng	6050300	1	6.98	1521760	20.0
Pentacosane	13.65	2.4	ng	188524	5	14.17	1565210	20.0
1-Chloroeicosane	13.98	4.1	ng	321138	5	14.17	1565210	20.0
Octacosane	14.30	3.3	ng	256311	5	14.17	1565210	20.0
Tricosane	14.61	3.5	ng	273566	5	14.17	1565210	20.0
Pentadecane, 8-he...	14.93	2.5	ng	196234	5	14.17	1565210	20.0
Heptacosane	15.29	3.1	ng	173115	6	15.71	1105260	20.0