

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071318\
 Data File : BF107392.D
 Acq On : 14 Jul 2018 3:35
 Operator : JU/SJ
 Sample : J3970-06
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 071118-DBRI-F-U-S

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-BF061918.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	5.154	476	479	490	rBV	12458	16843	1.06%	0.215%
2	5.566	546	549	573	rBV	244440	330435	20.86%	4.210%
3	6.578	718	721	739	rBV2	167232	240397	15.17%	3.063%
4	6.701	739	742	752	rBV	569177	582145	36.74%	7.417%
5	6.925	777	780	788	rBV	249278	220652	13.93%	2.811%
6	7.084	803	807	816	rBV	843342	751883	47.46%	9.579%
7	7.495	873	877	893	rBV	639813	622168	39.27%	7.927%
8	8.213	995	999	1018	rBV	216040	241909	15.27%	3.082%
9	9.284	1177	1181	1197	rBV	1078126	1103236	69.64%	14.055%
10	9.684	1246	1249	1264	rBV	121278	117990	7.45%	1.503%
11	9.972	1295	1298	1310	rVB	250834	263700	16.64%	3.360%
12	10.636	1408	1411	1418	rBB	36489	34367	2.17%	0.438%
13	10.772	1431	1434	1447	rBV	437108	489060	30.87%	6.231%
14	11.472	1550	1553	1567	rBB	322390	317835	20.06%	4.049%
15	13.060	1818	1823	1826	rBV	1558209	1584300	100.00%	20.184%
16	13.254	1853	1856	1862	rBV	15046	15967	1.01%	0.203%
17	13.595	1911	1914	1917	rBV	25552	24137	1.52%	0.308%
18	13.930	1967	1971	1972	rBV	30782	29885	1.89%	0.381%
19	13.954	1972	1975	1985	rVB3	22951	45686	2.88%	0.582%
20	14.130	2001	2005	2013	rVB	350384	332688	21.00%	4.239%
21	14.242	2021	2024	2029	rVB	43977	38461	2.43%	0.490%
22	14.548	2071	2076	2081	rBV	49934	48022	3.03%	0.612%
23	14.866	2126	2130	2135	rVB	44979	45240	2.86%	0.576%
24	15.213	2185	2189	2193	rBV	40248	42725	2.70%	0.544%
25	15.607	2252	2256	2260	rBV	32139	39991	2.52%	0.509%
26	15.666	2261	2266	2280	rVB2	145125	219301	13.84%	2.794%
27	16.060	2328	2333	2339	rBV	20949	33182	2.09%	0.423%
28	16.595	2419	2424	2428	rVB3	10270	16940	1.07%	0.216%

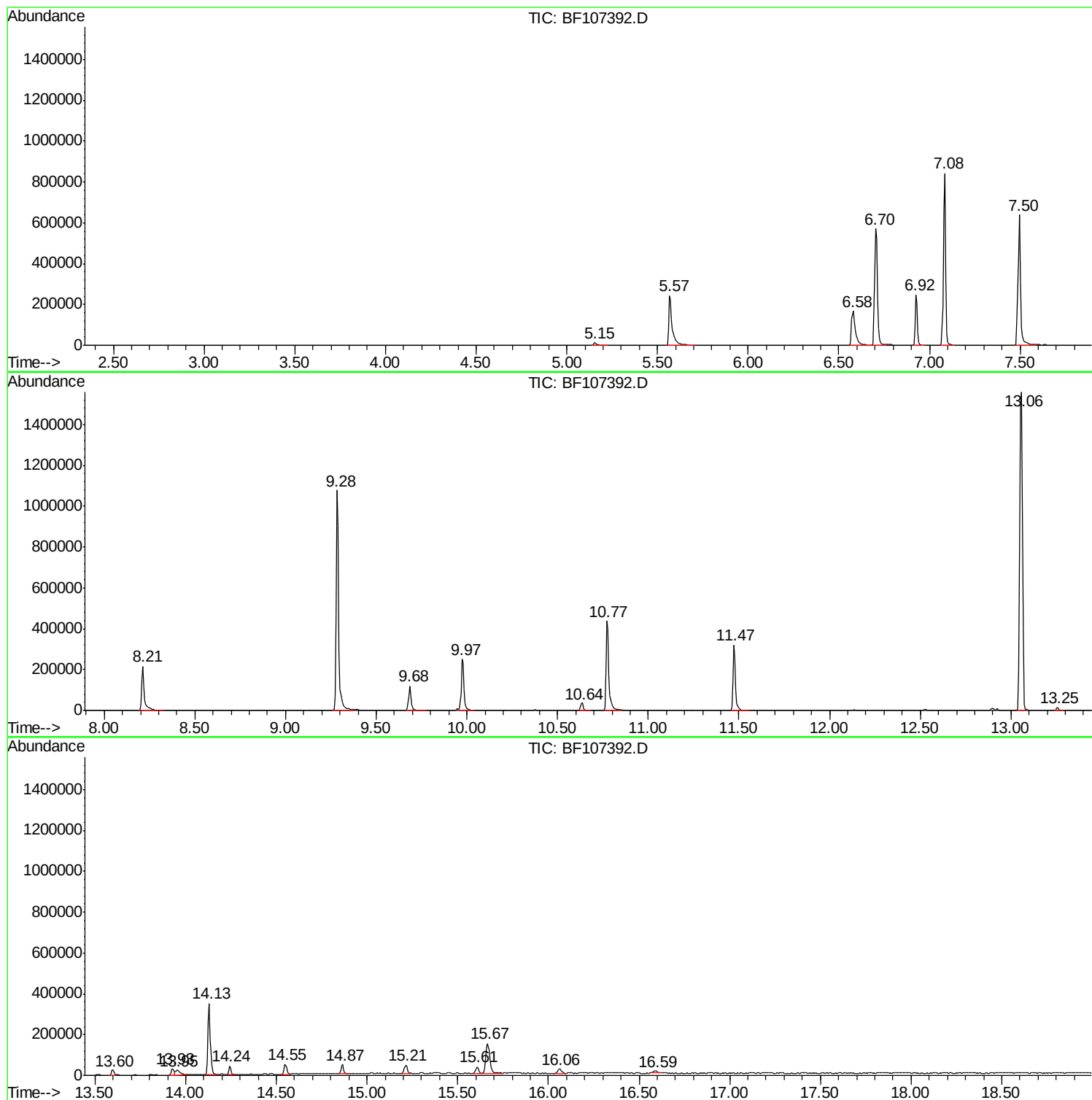
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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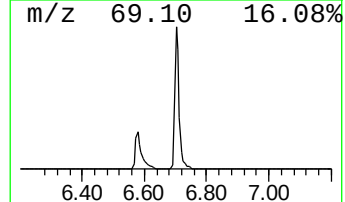
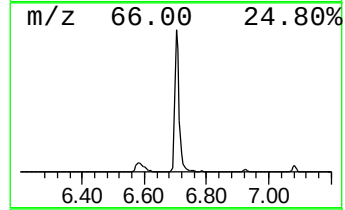
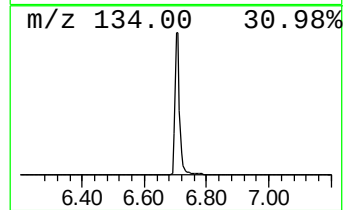
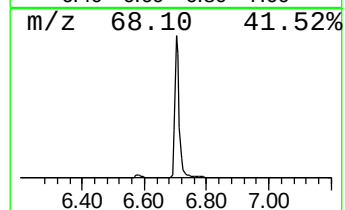
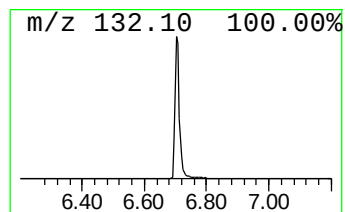
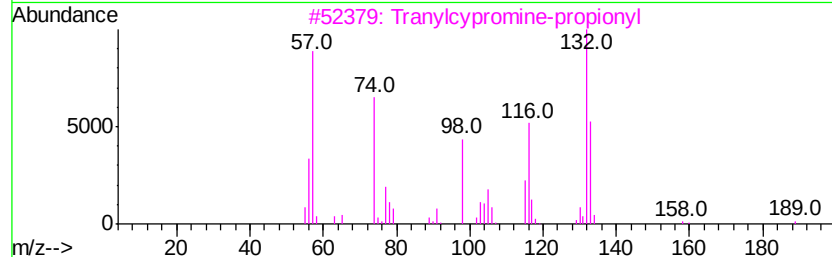
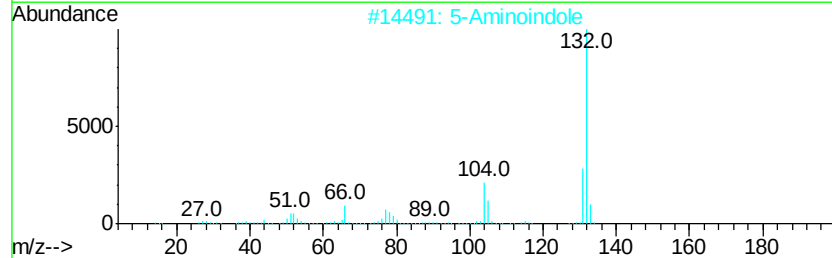
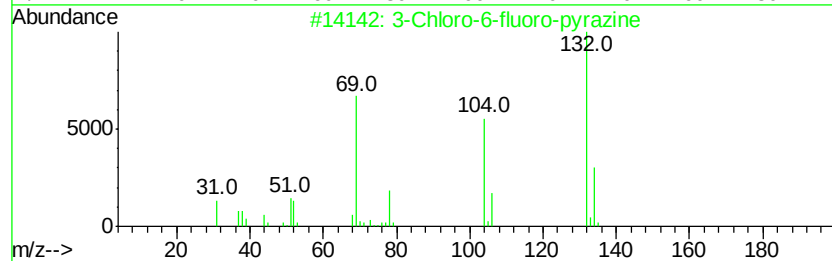
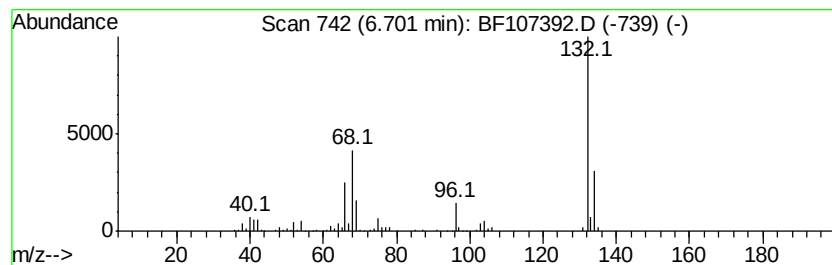
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	52.77 ng	582145	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	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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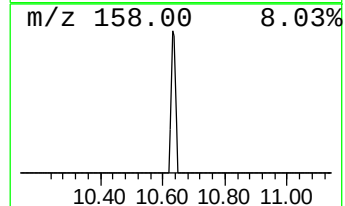
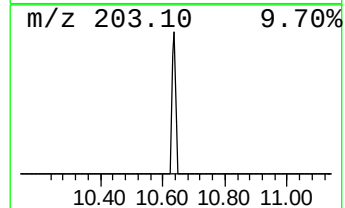
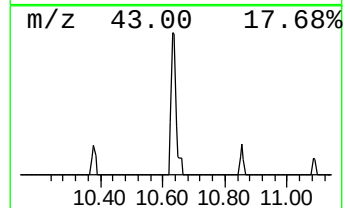
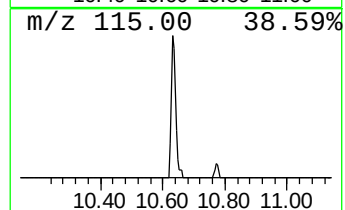
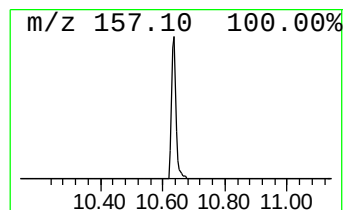
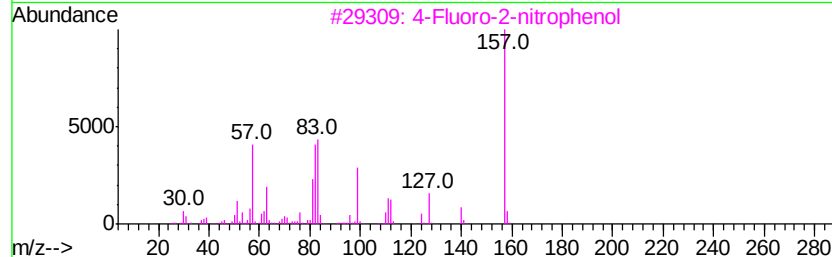
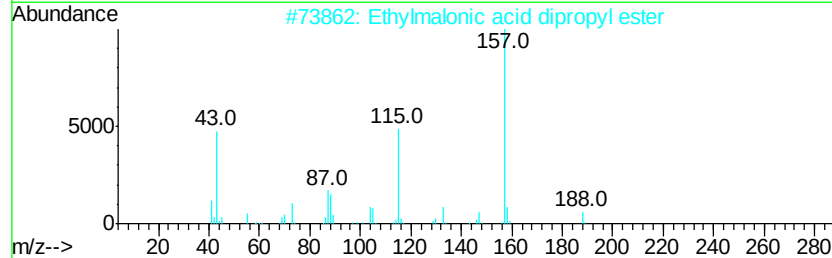
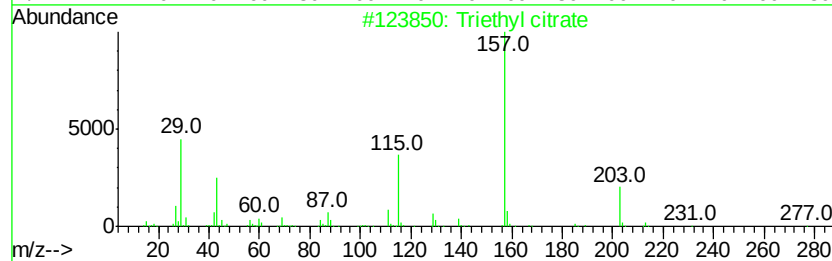
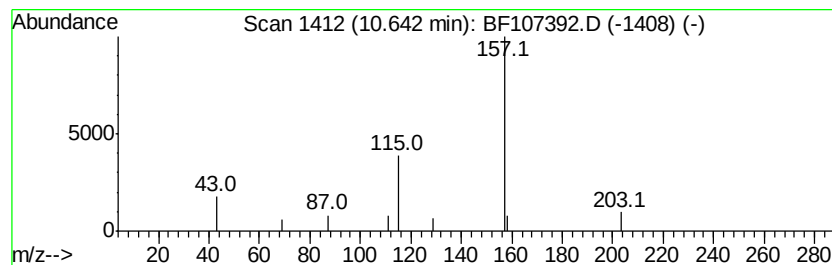
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Peak Number 3 Triethyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.61 ng	34367	Acenaphthene-d10	9.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triethyl citrate	276	C12H20O7	000077-93-0	86
2			Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	45
3			4-Fluoro-2-nitrophenol	157	C6H4FN03	000394-33-2	40
4			Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	36
5			5-Chloro-2,6-dimethyl-4-pyrimidi...	157	C6H8ClN3	002858-20-0	9



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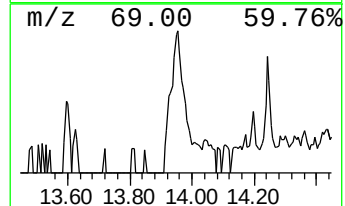
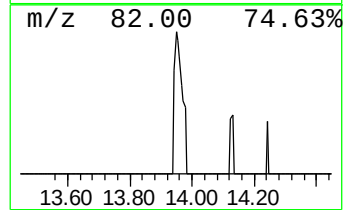
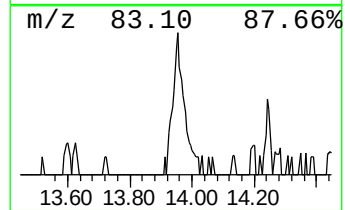
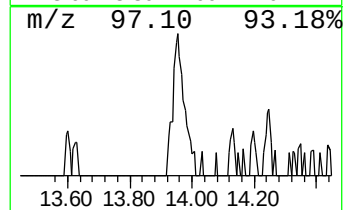
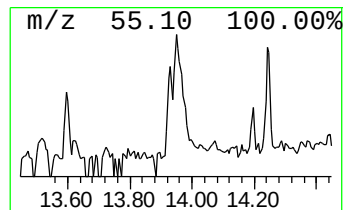
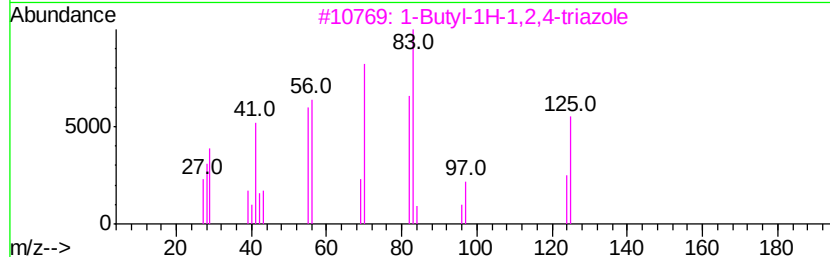
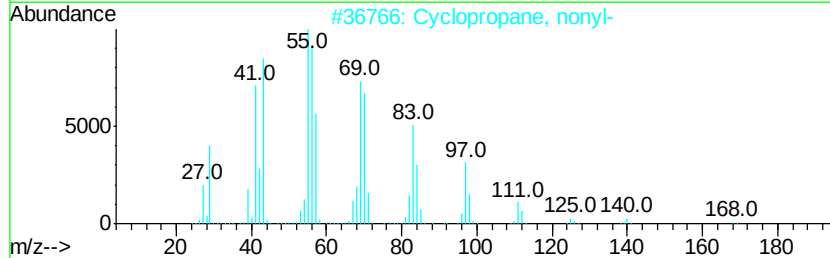
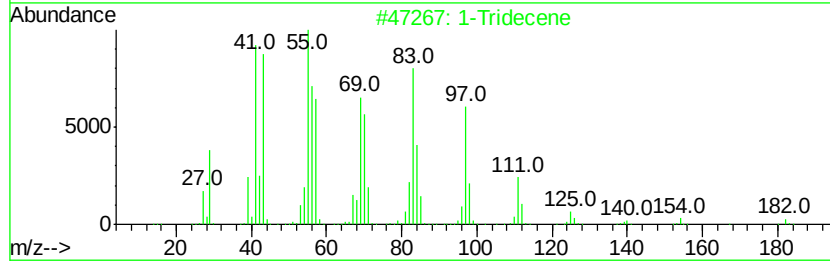
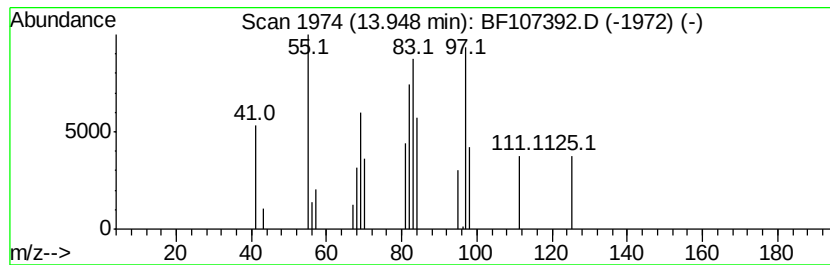
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Peak Number 4 unknown13.95 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.75 ng	45686	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tridecene	182	C13H26	002437-56-1	33
2		Cyclopropane, nonyl-	168	C12H24	074663-85-7	20
3		1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	16
4		Cyclohexane, methyl-	98	C7H14	000108-87-2	16
5		Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	12



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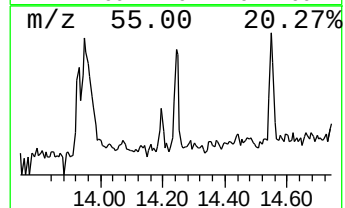
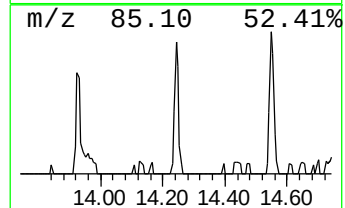
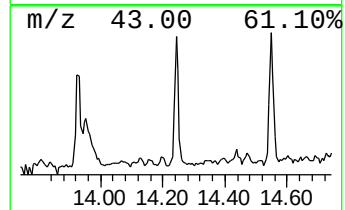
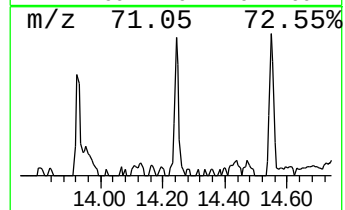
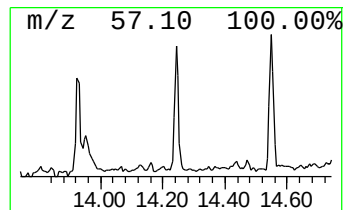
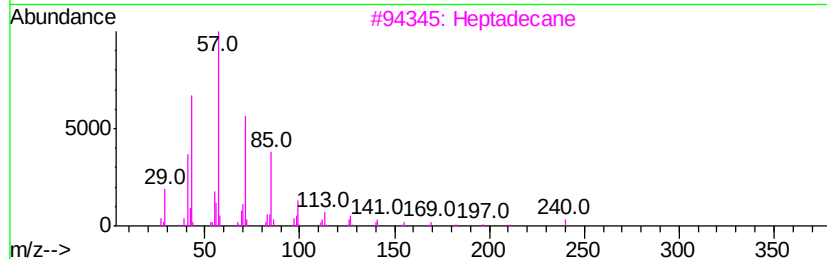
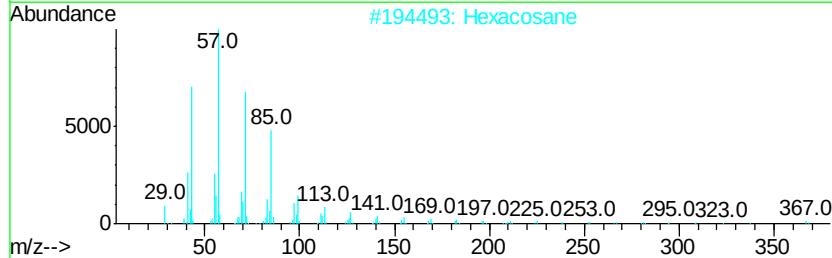
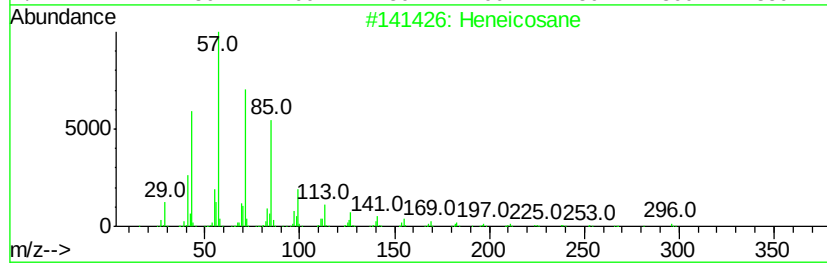
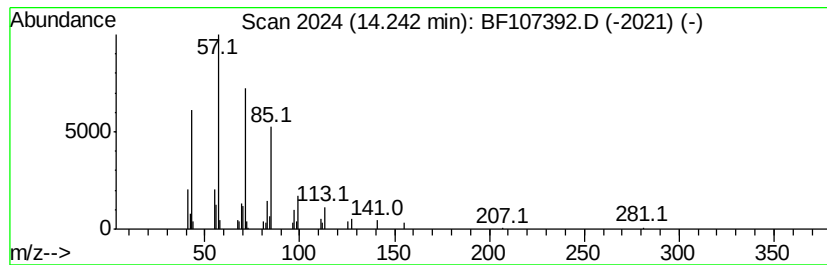
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Peak Number 5 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.31 ng	38461	Chrysene-d12	14.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	90
3	Heptadecane		240	C17H36	000629-78-7	86
4	Nonadecane		268	C19H40	000629-92-5	86
5	Octadecane		254	C18H38	000593-45-3	86



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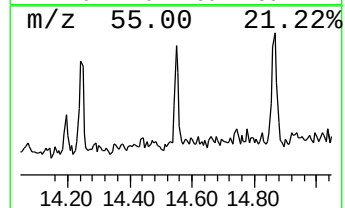
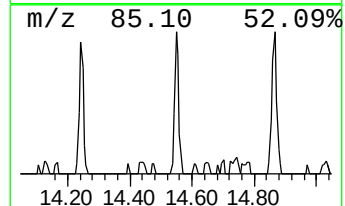
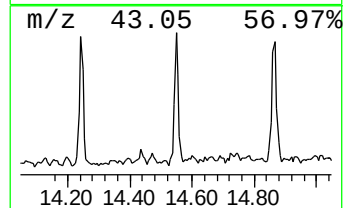
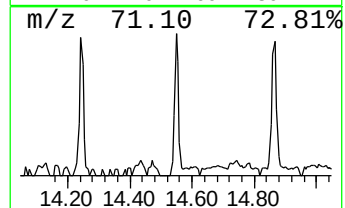
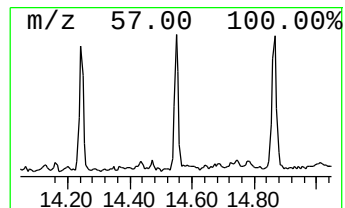
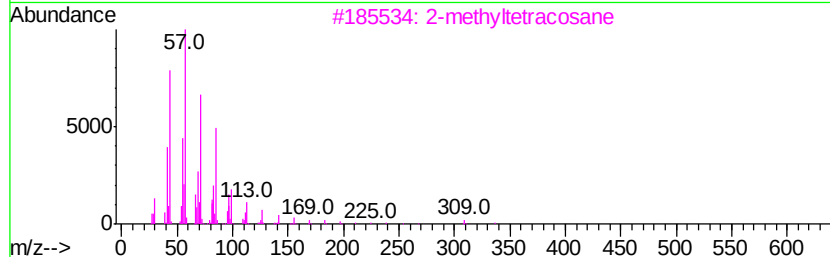
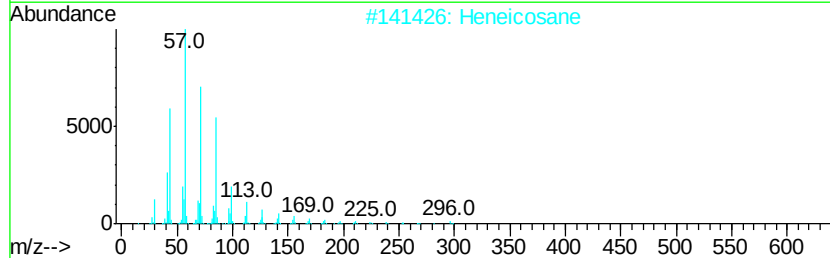
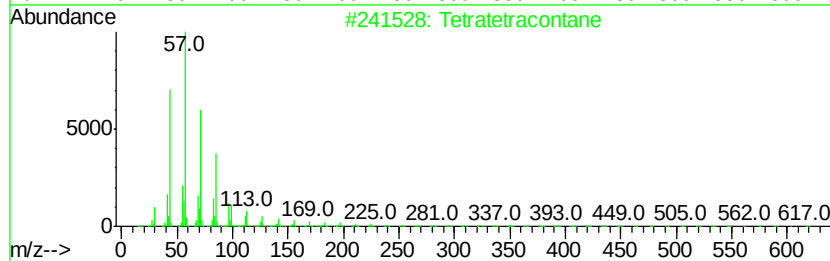
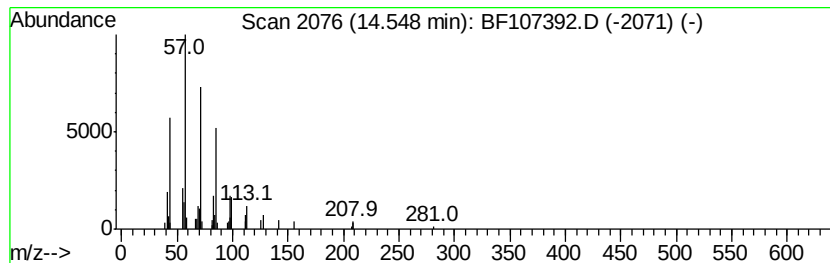
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Peak Number 6 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.89 ng	48022	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		2-methyltetracosane	352	C25H52	1000376-72-6	90
4		Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



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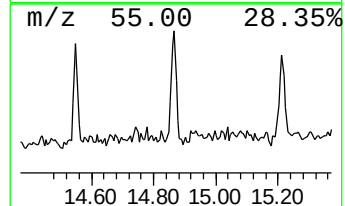
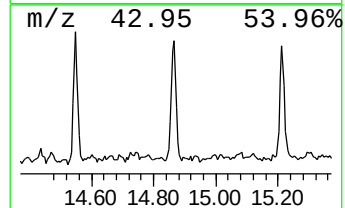
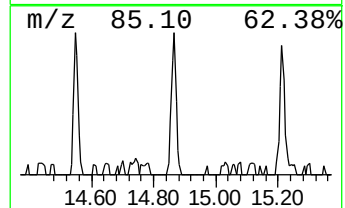
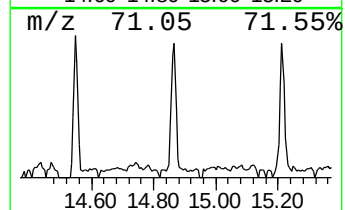
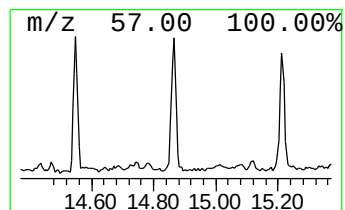
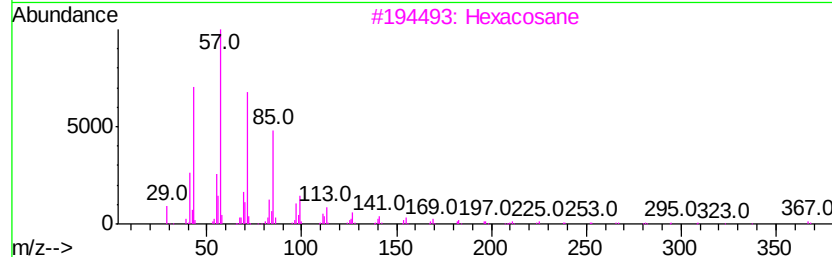
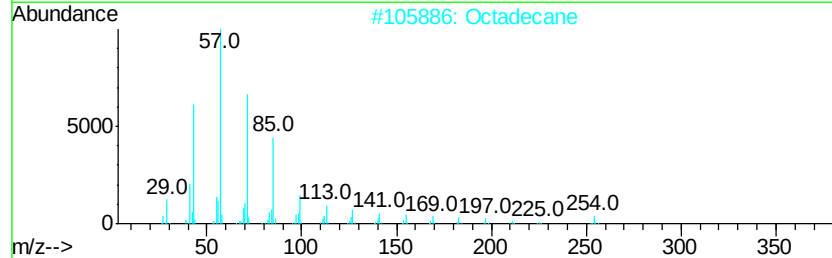
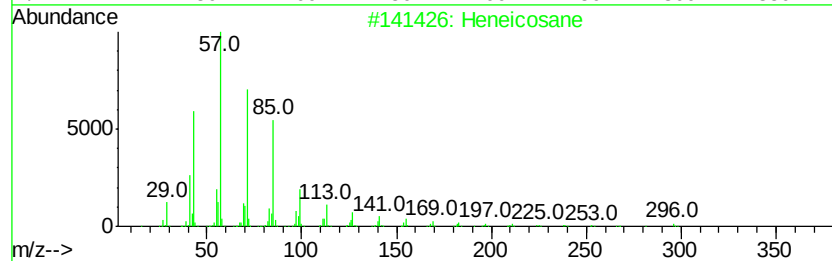
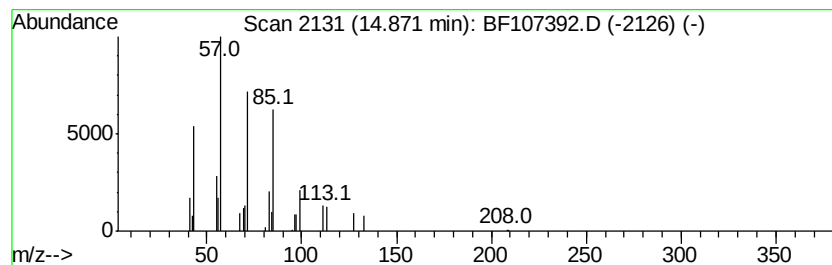
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.72 ng	45240	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Octadecane	254	C18H38	000593-45-3	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107392.D
Acq On : 14 Jul 2018 3:35
Operator : JU/SJ
Sample : J3970-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
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ClientSampleId :
071118-DBRI-F-U-S

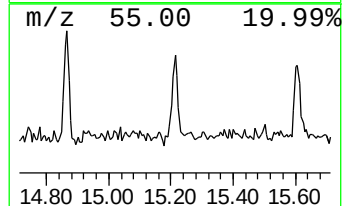
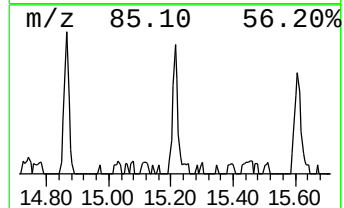
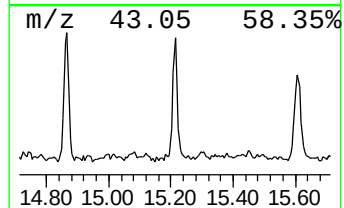
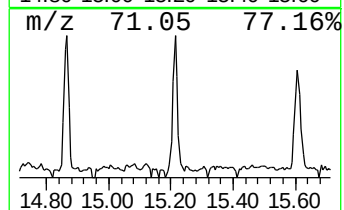
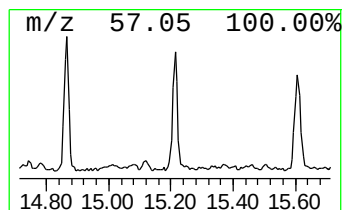
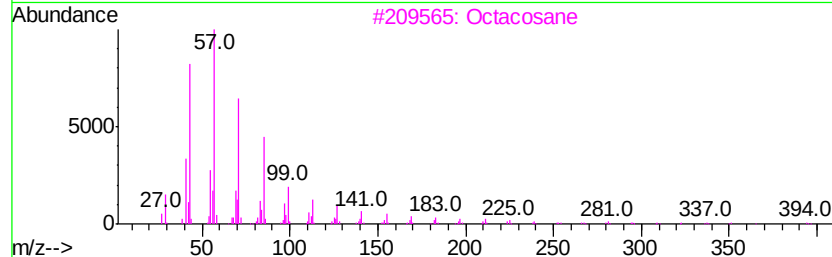
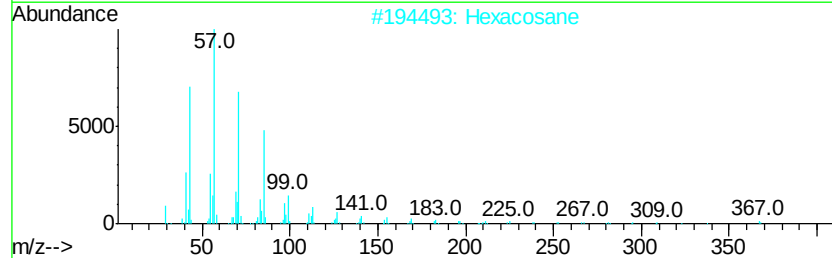
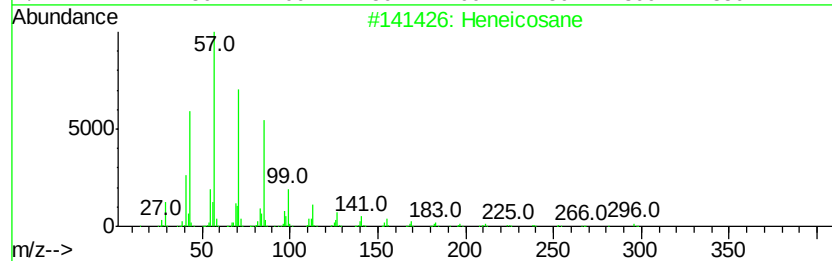
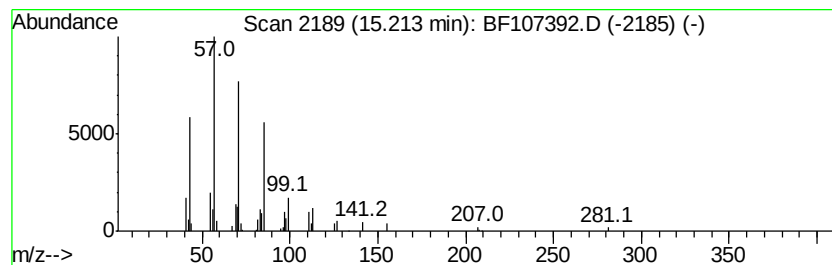
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	3.90 ng	42725	Perylene-d12	15.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	90
3	Octacosane		394	C28H58	000630-02-4	90
4	Pentacosane		352	C25H52	000629-99-2	90
5	Heptadecane		240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107392.D
Acq On : 14 Jul 2018 3:35
Operator : JU/SJ
Sample : J3970-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
071118-DBRI-F-U-S

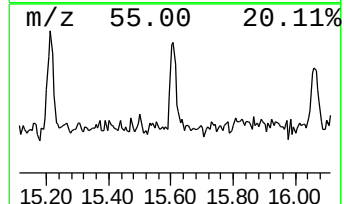
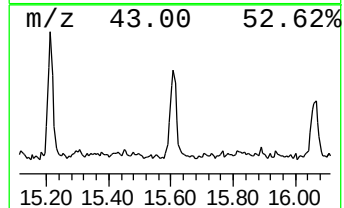
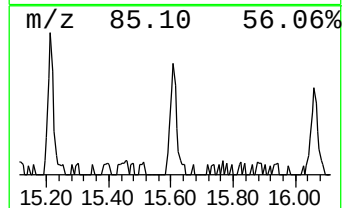
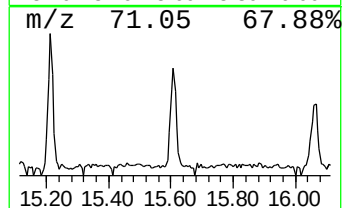
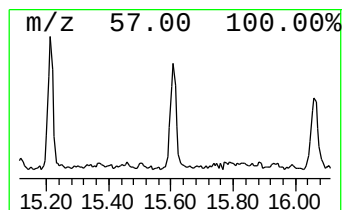
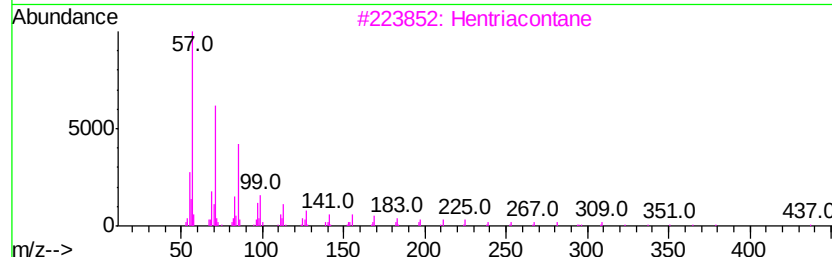
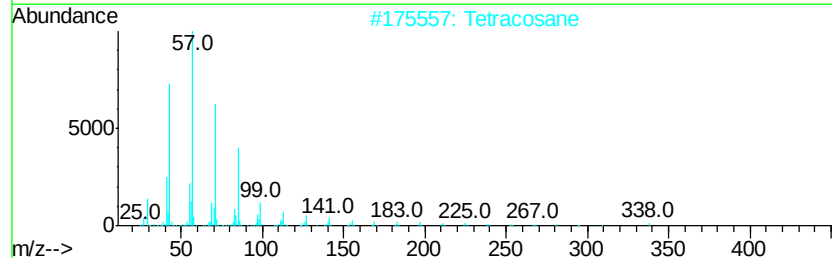
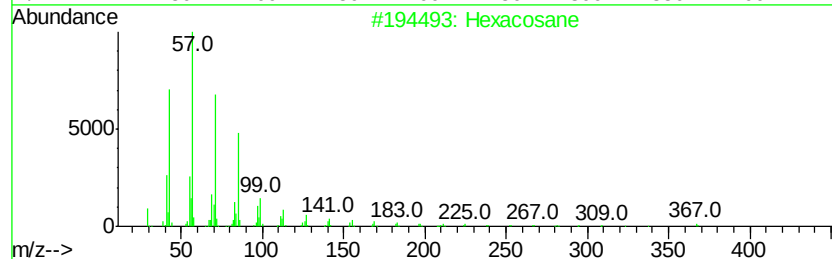
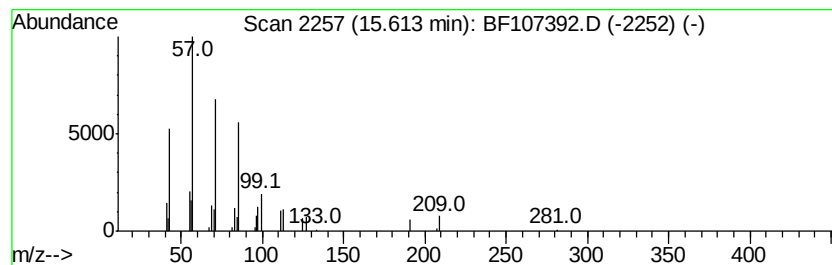
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	3.65 ng	39991	Perylene-d12	15.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	87
2	Tetracosane		338	C24H50	000646-31-1	87
3	Hentriacontane		437	C31H64	000630-04-6	87
4	Tetratetracontane		619	C44H90	007098-22-8	87
5	Heptacosane		380	C27H56	000593-49-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071318\
Data File : BF107392.D
Acq On : 14 Jul 2018 3:35
Operator : JU/SJ
Sample : J3970-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
071118-DBRI-F-U-S

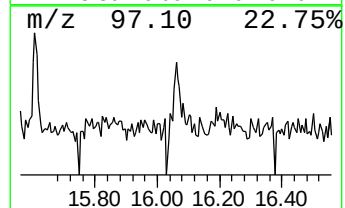
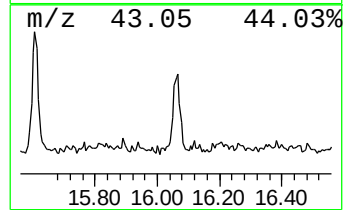
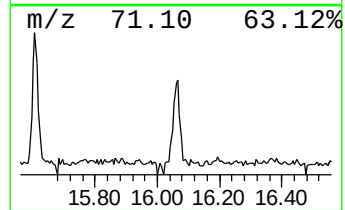
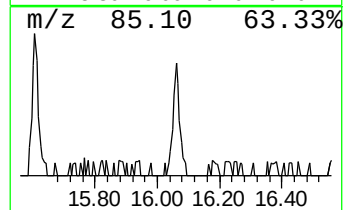
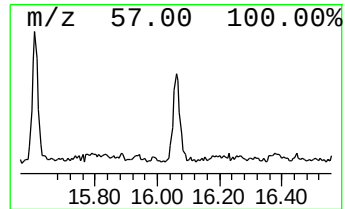
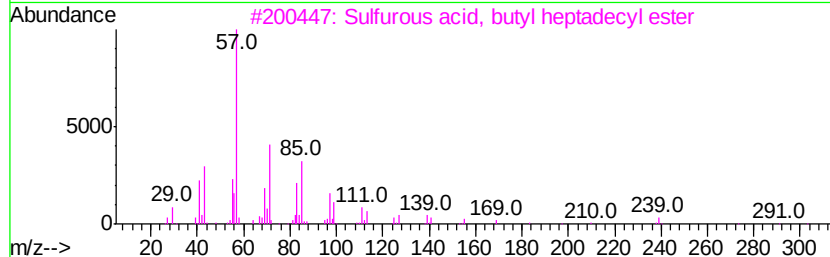
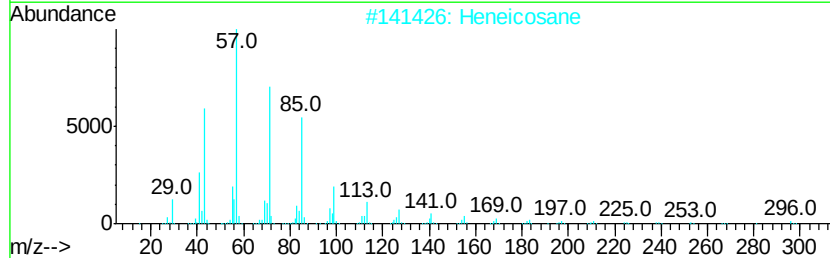
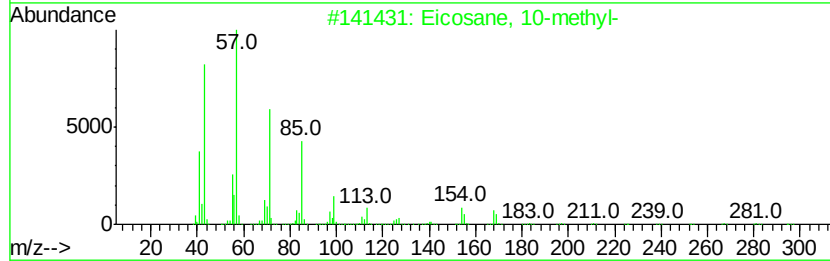
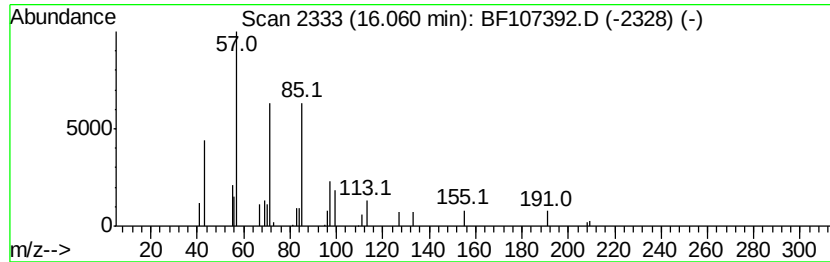
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane, 10-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	3.03 ng	33182	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
2		Heneicosane	296	C21H44	000629-94-7	80
3		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	78
4		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	78
5		Heptadecane	240	C17H36	000629-78-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071318\
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Operator : JU/SJ
Sample : J3970-06
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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Triethyl citrate	10.64	2.6	ng	34367	3	9.97	263700	20.0
unknown13.95	13.95	2.8	ng	45686	5	14.13	332688	20.0
Heneicosane	14.24	2.3	ng	38461	5	14.13	332688	20.0
Tetratetracontane	14.55	2.9	ng	48022	5	14.13	332688	20.0
Octadecane	14.87	2.7	ng	45240	5	14.13	332688	20.0
Pentacosane	15.21	3.9	ng	42725	6	15.67	219301	20.0
Hexacosane	15.61	3.6	ng	39991	6	15.67	219301	20.0
Eicosane, 10-methyl-	16.06	3.0	ng	33182	6	15.67	219301	20.0