LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118236.D
Acq On : 17 Dec 2019 19:51
Operator : JU
Sample : K6327-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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-BF120619.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	2.134	3	8	14	rVB	316387	399802	13.10%	1.464%
2	5.075	503	508	523	rVB	370008	478976	15.69%	1.753%
3	5.481	573	577	580	rBV	2853655	2563356	83.99%	9.384%
4	6.492	744	749	768	rBV	2485018	2841724	93.11%	10.403%
5	6.634	768	773	776	rBV	3308373	2995373	98.15%	10.965%
6	6.857	808	811	820	rBV	873931	747071	24.48%	2.735%
7	7.016	834	838	842	rBV	2744458	2318009	75.95%	8.485%
8	7.428	903	908	911	rBV	1774721	1687772	55.30%	6.178%
9	8.145	1026	1030	1051	rBV	1046620	948011	31.06%	3.470%
10	9.228	1209	1214	1217	rBV	3513078	3051913	100.00%	11.172%
11	9.622	1277	1281	1289	rBV	133899	132603	4.34%	0.485%
12	9.910	1326	1330	1343	rBV	1155200	1029953	33.75%	3.770%
13	10.704	1460	1465	1475	rBV	1877119	1797892	58.91%	6.581%
14	11.404	1580	1584	1591	rBV	916793	881275	28.88%	3.226%
15	11.921	1669	1672	1687	rBV	193510	229930	7.53%	0.842%
16	12.621	1788	1791	1804	rBV	40017	50061	1.64%	0.183%
17	12.710	1804	1806	1817	rBV2	47886	71632	2.35%	0.262%
18	12.992	1850	1854	1857	rBV	2759926	2346945	76.90%	8.591%
19	13.216	1887	1892	1895	rVB2	30534	34778	1.14%	0.127%
20	13.563	1946	1951	1958	rBV2	42699	53498	1.75%	0.196%
21	13.886	2002	2006	2018	rBV	351818	486985	15.96%	1.783%
22	14.057	2030	2035	2043	rBV	764069	826387	27.08%	3.025%
23	14.210	2057	2061	2065	rBV	76172	82755	2.71%	0.303%
24	14.515	2110	2113	2121	rBV2	90521	126133	4.13%	0.462%
25	14.827	2160	2166	2169	rVB2	89709	114862	3.76%	0.420%
26	14.898	2175	2178	2183	rBV	72466	81129	2.66%	0.297%
27	15.168	2220	2224	2229	rBV	85246	98710	3.23%	0.361%
28	15.545	2283	2288	2297	rBV	519615	748784	24.53%	2.741%
29	15.998	2362	2365	2371	rVB	62155	91206	2.99%	0.334%

Sum of corrected areas: 27317525

LSC Report - Integrated Chromatogram

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Acq On : 17 Dec 2019 19:51
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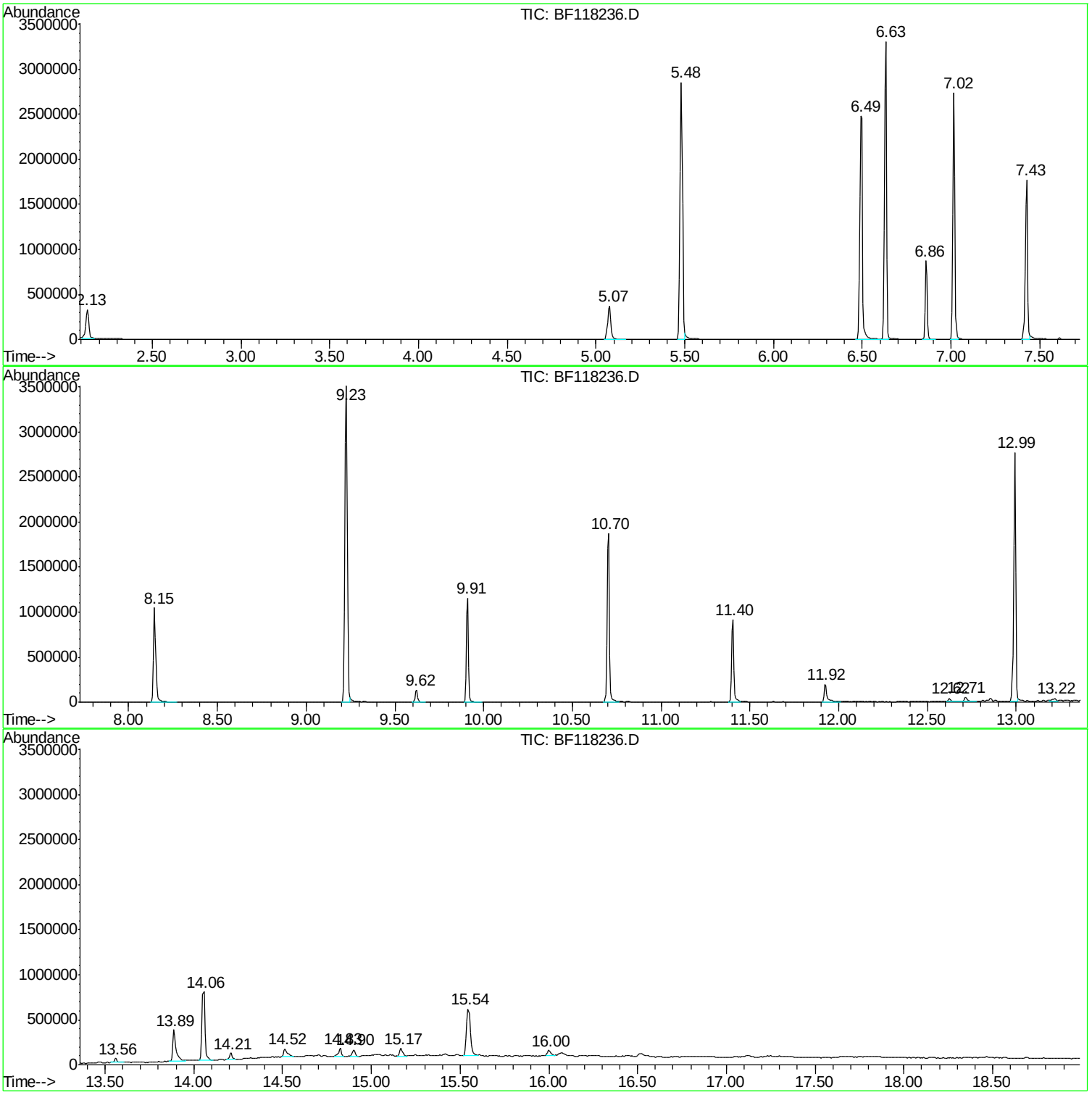
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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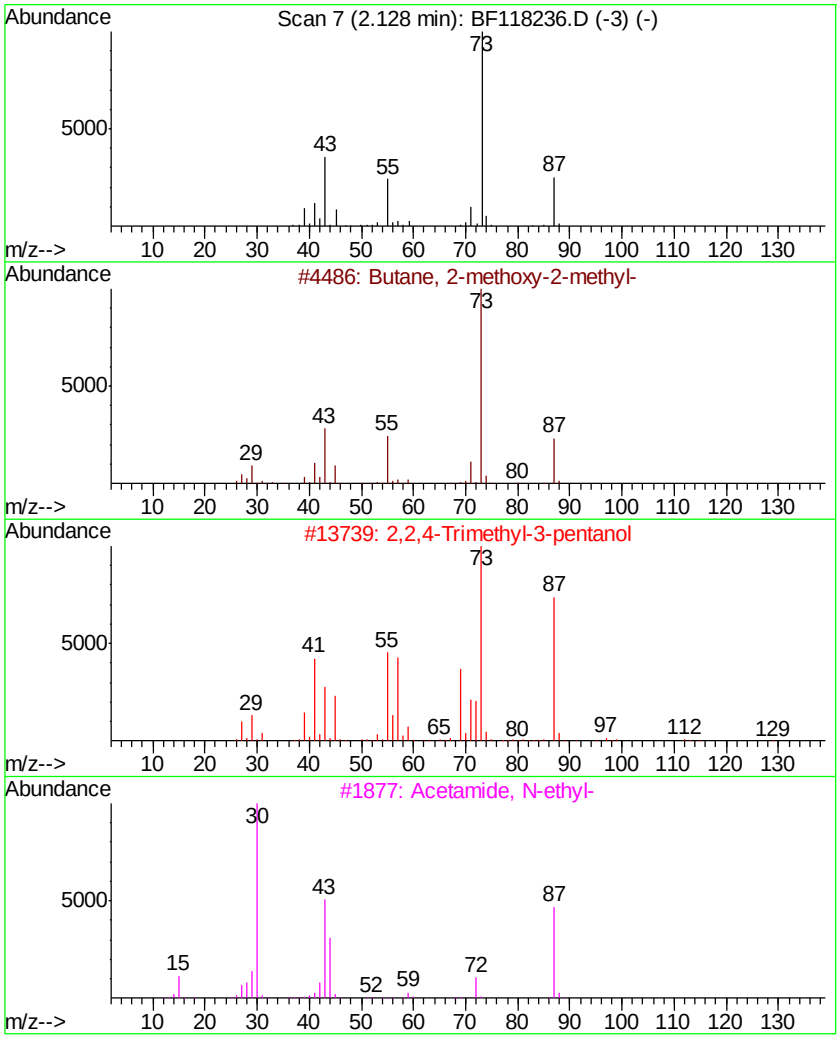
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

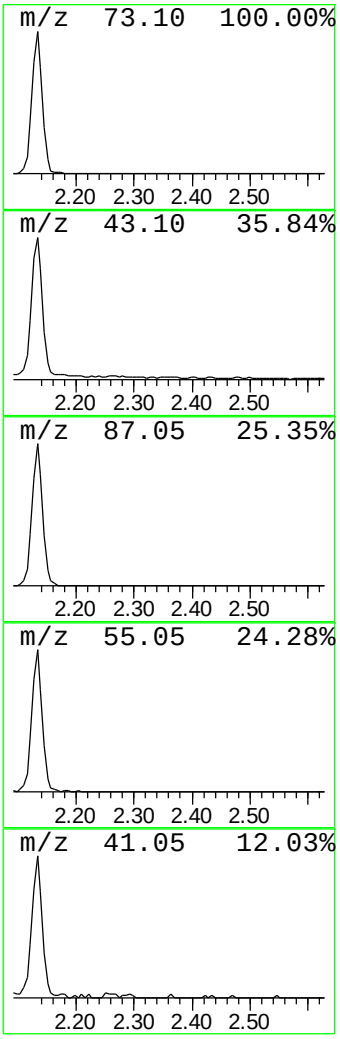
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	10.70 ng	399802	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Misc :
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Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

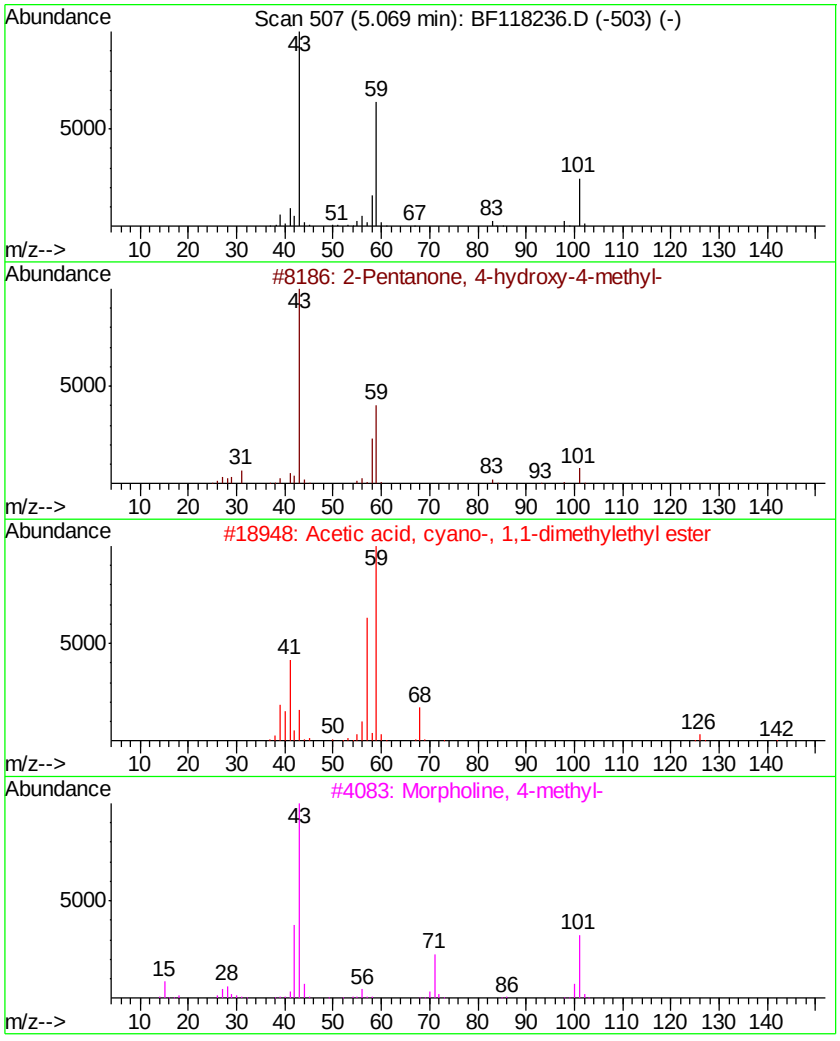
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

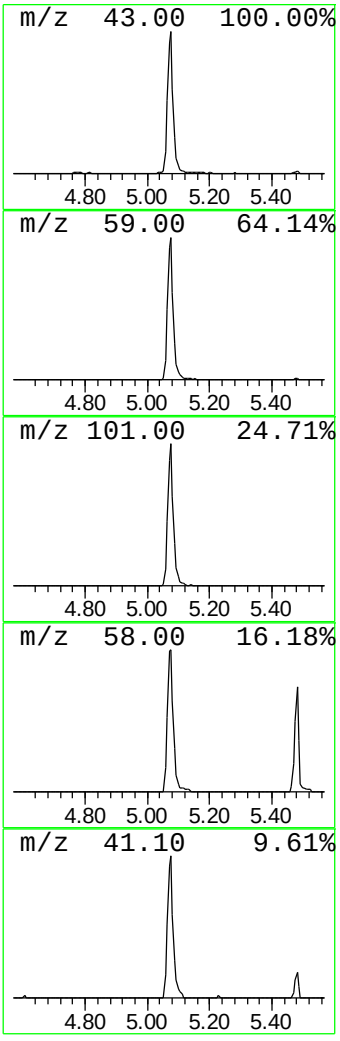
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.82 ng	478976	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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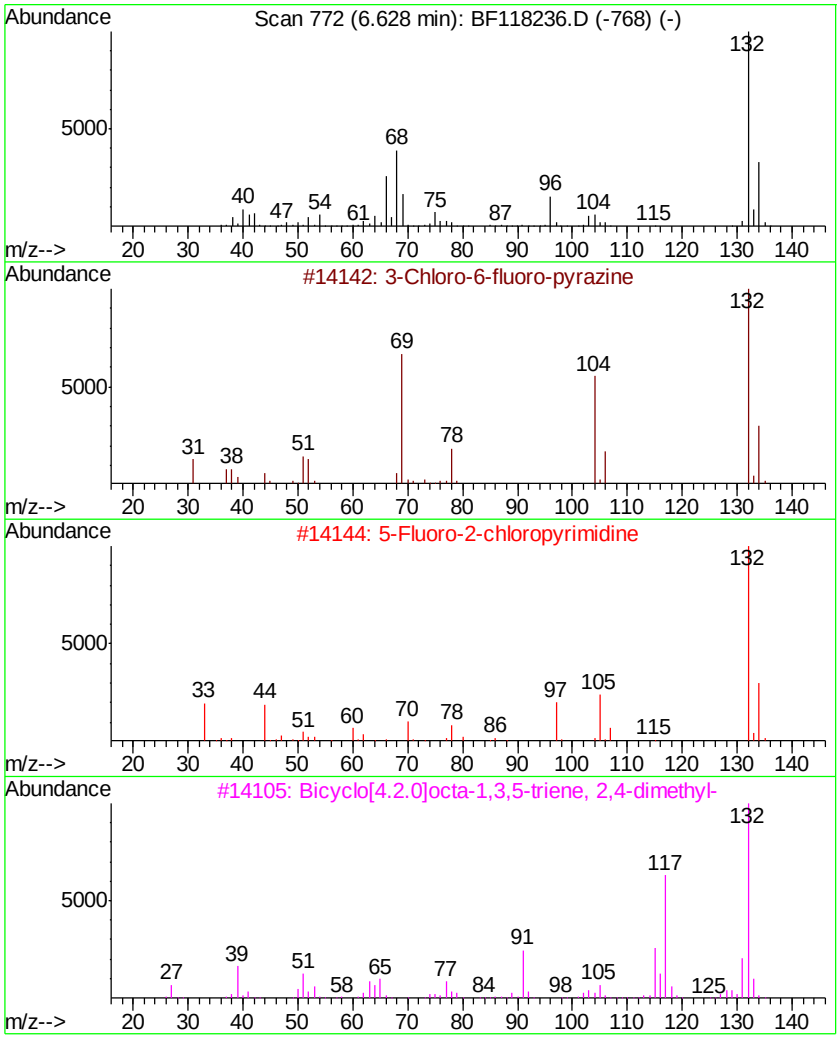
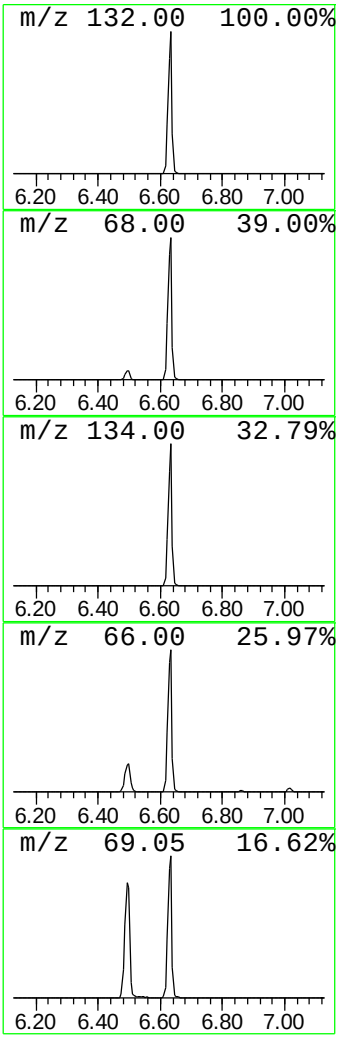
Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.19 ng	2995370	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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TIC Library : C:\DATABASE\NIST11.L
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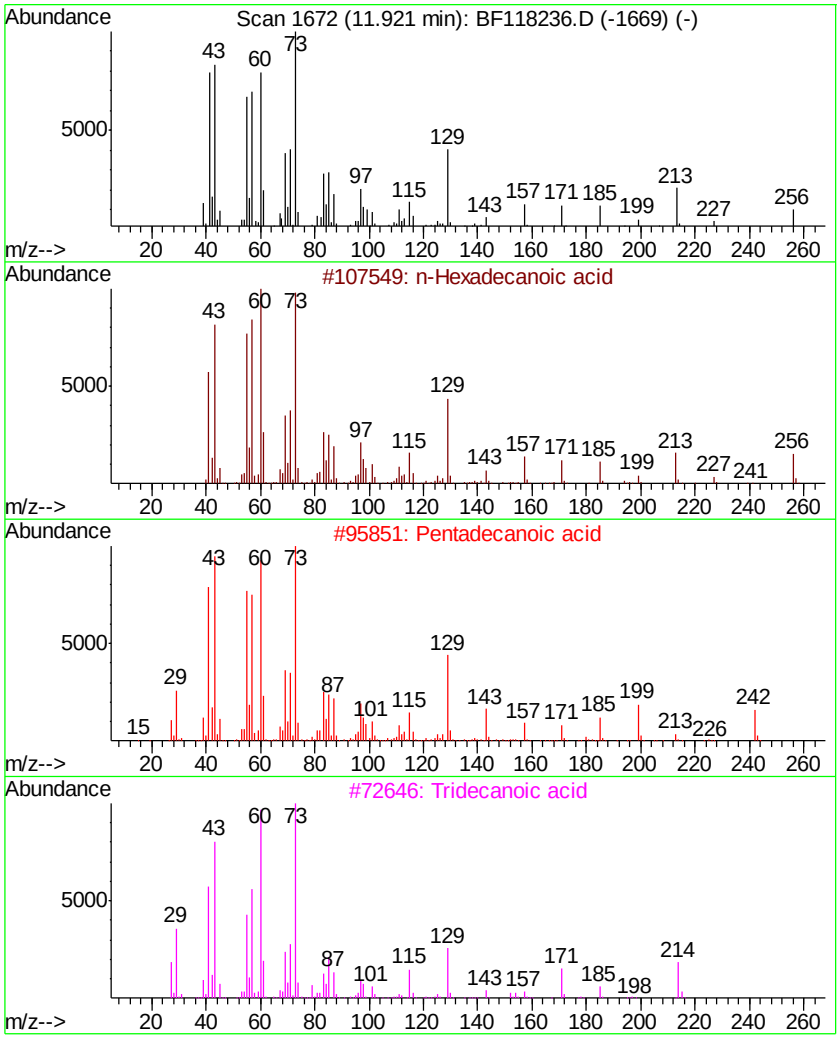
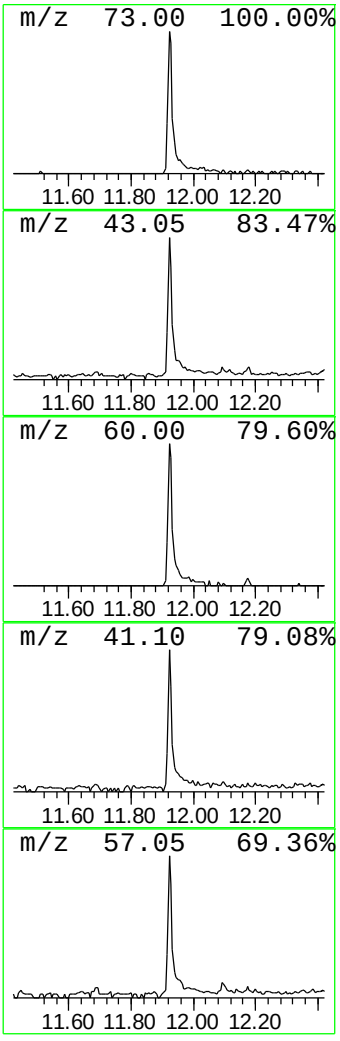
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.22 ng	229930	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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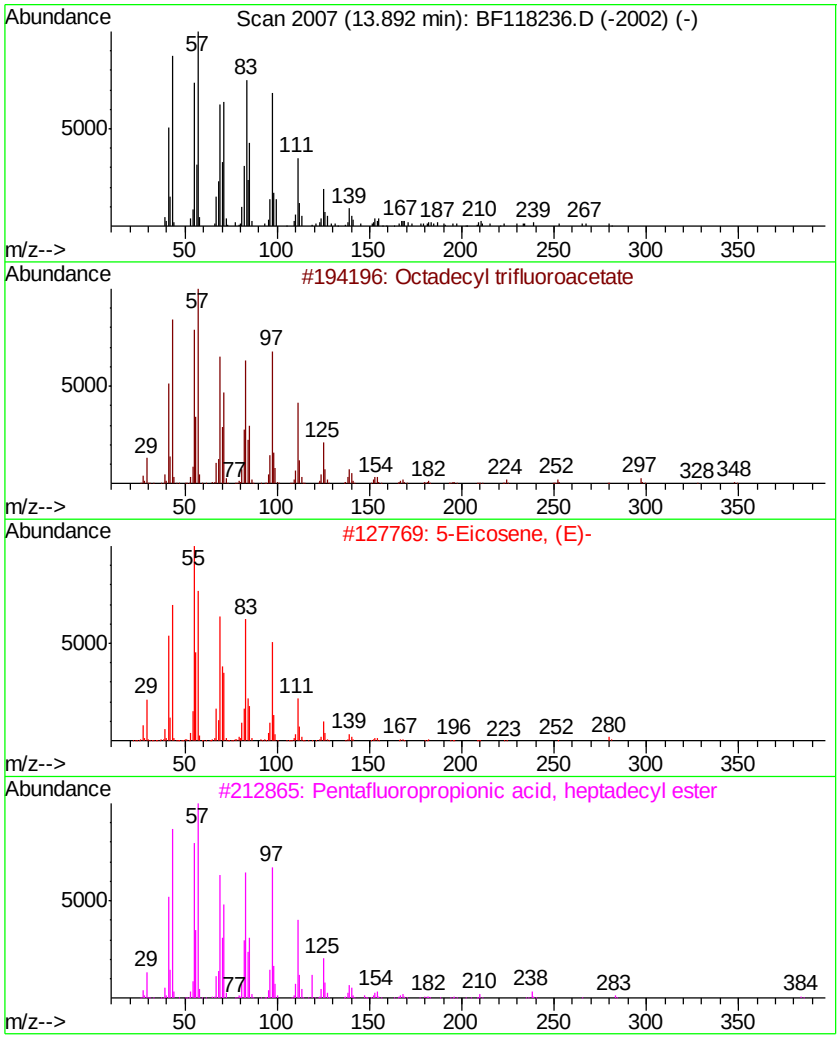
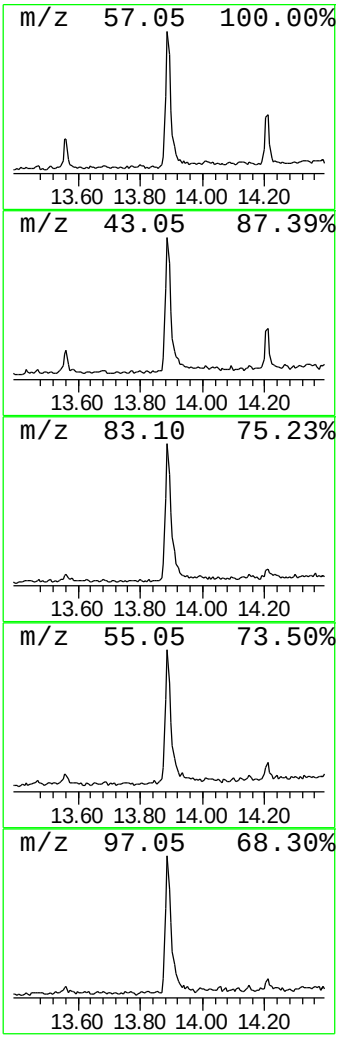
****

Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	11.79 ng	486985	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94





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Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

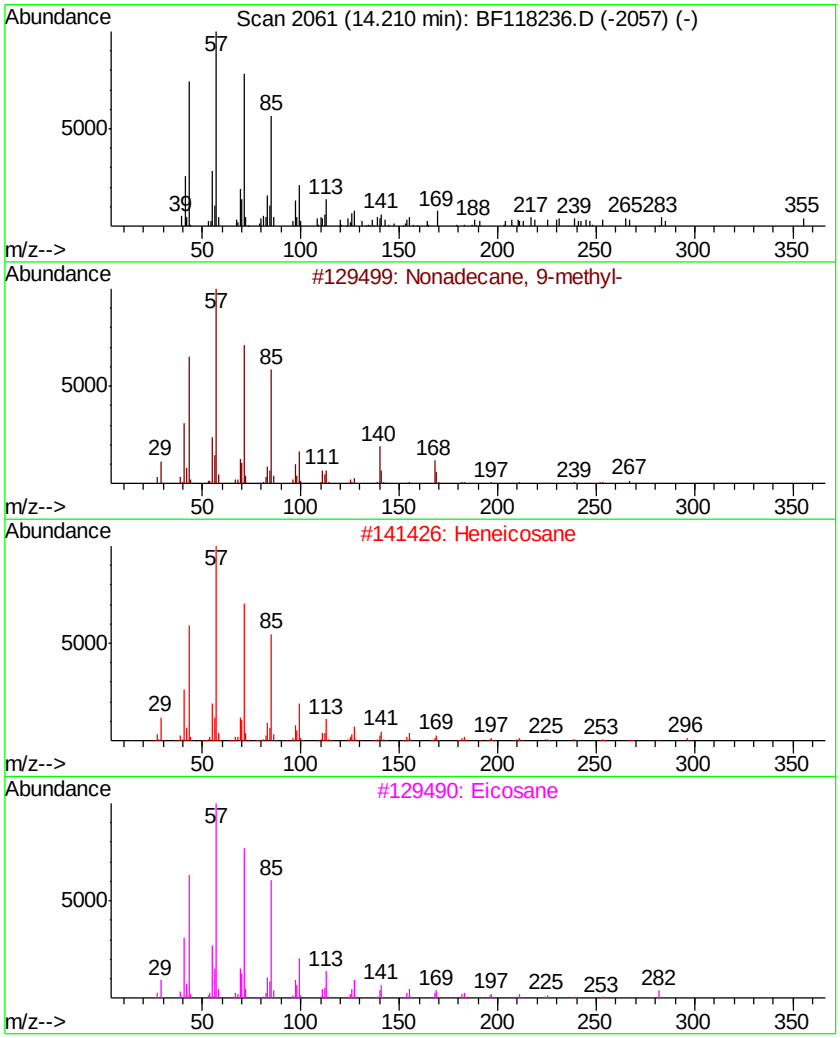
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

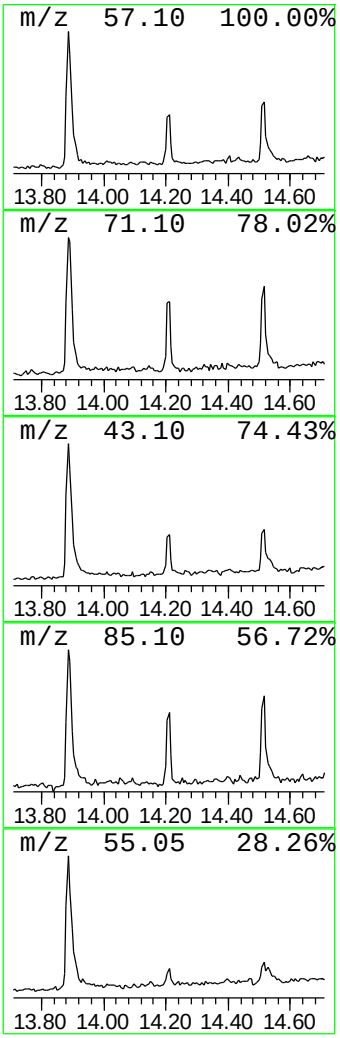
****

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.00 ng	82755	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Hentriacontane	437	C31H64	000630-04-6	87





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Misc :
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Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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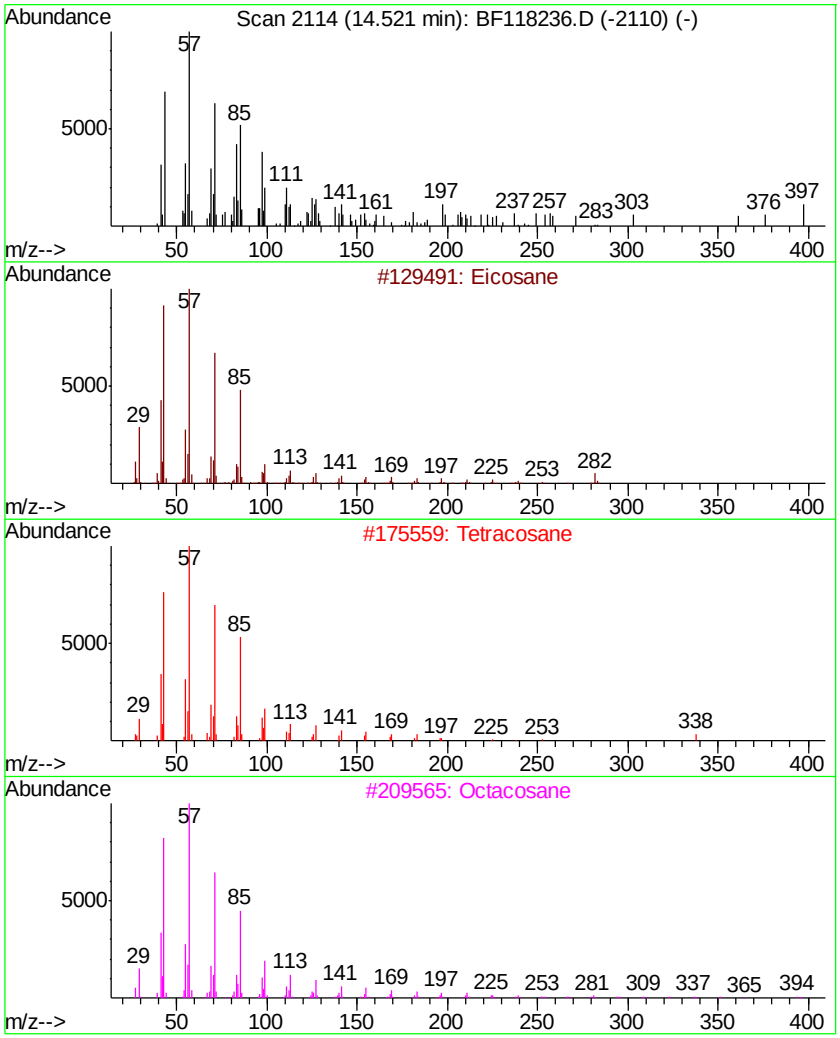
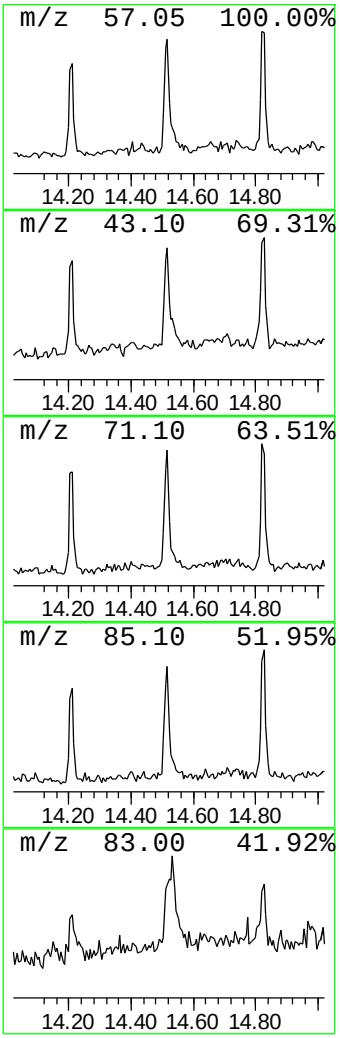
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.05 ng	126133	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





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TIC Library : C:\DATABASE\NIST11.L
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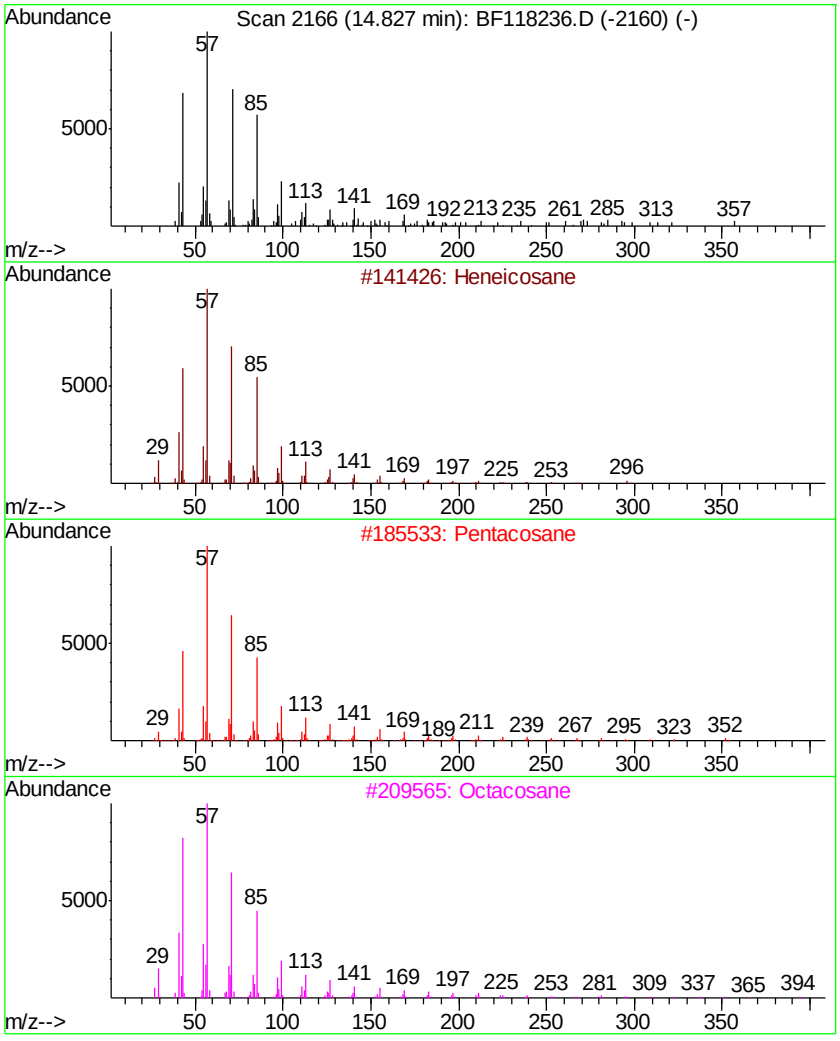
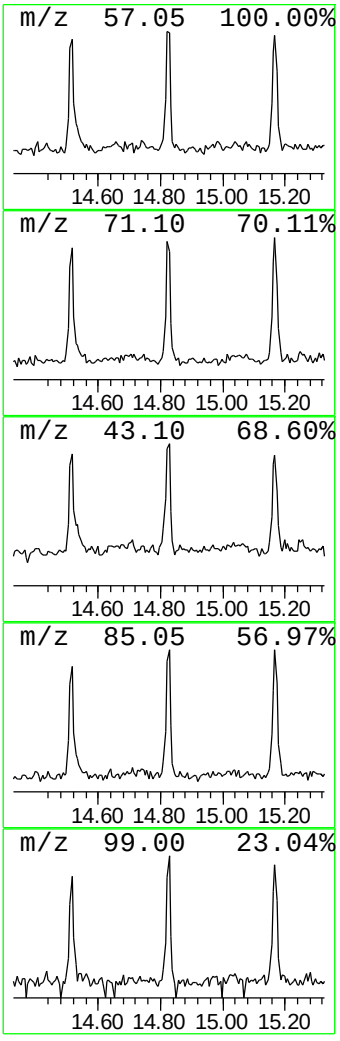
Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.07 ng	114862	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Docosane	310	C22H46	000629-97-0	91
5	Triacontane	422	C30H62	000638-68-6	90





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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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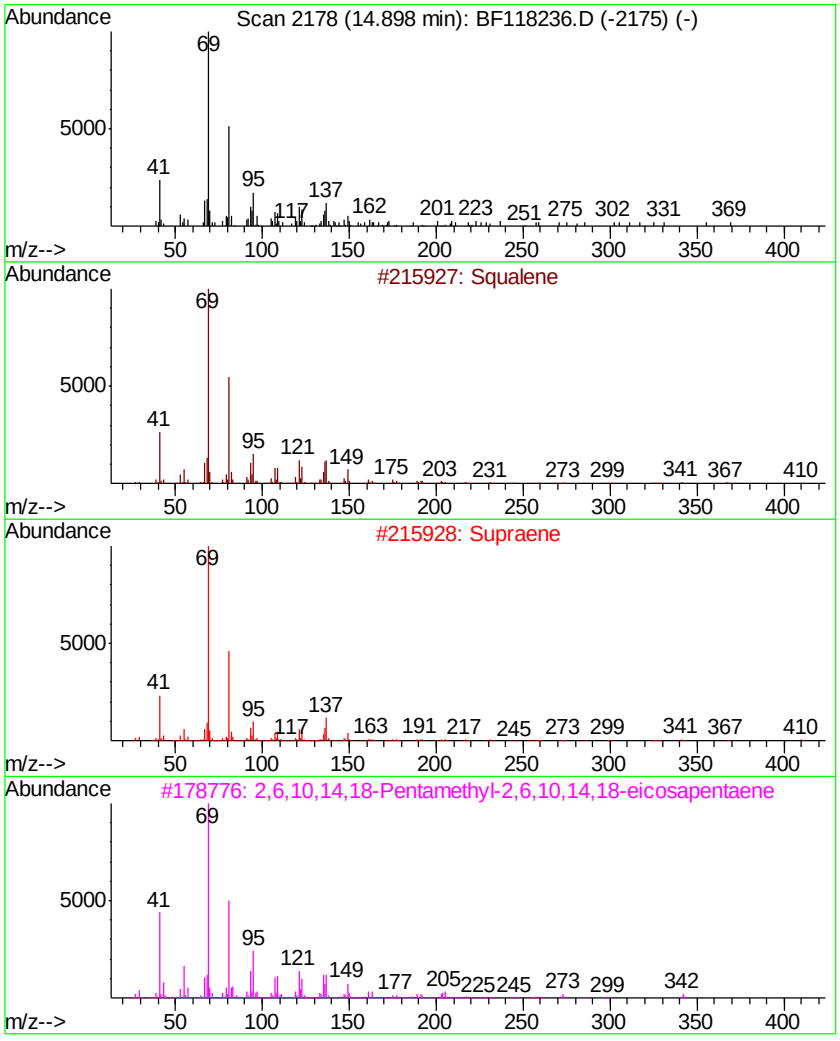
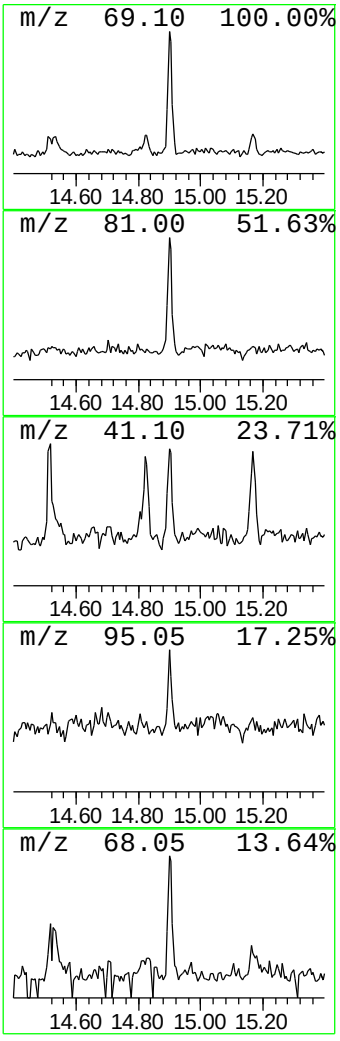
Peak Number 10 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.17 ng	81129	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	83
2	Supraene	410	C30H50	007683-64-9	80
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118236.D
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Misc :
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Instrument : BNA_F
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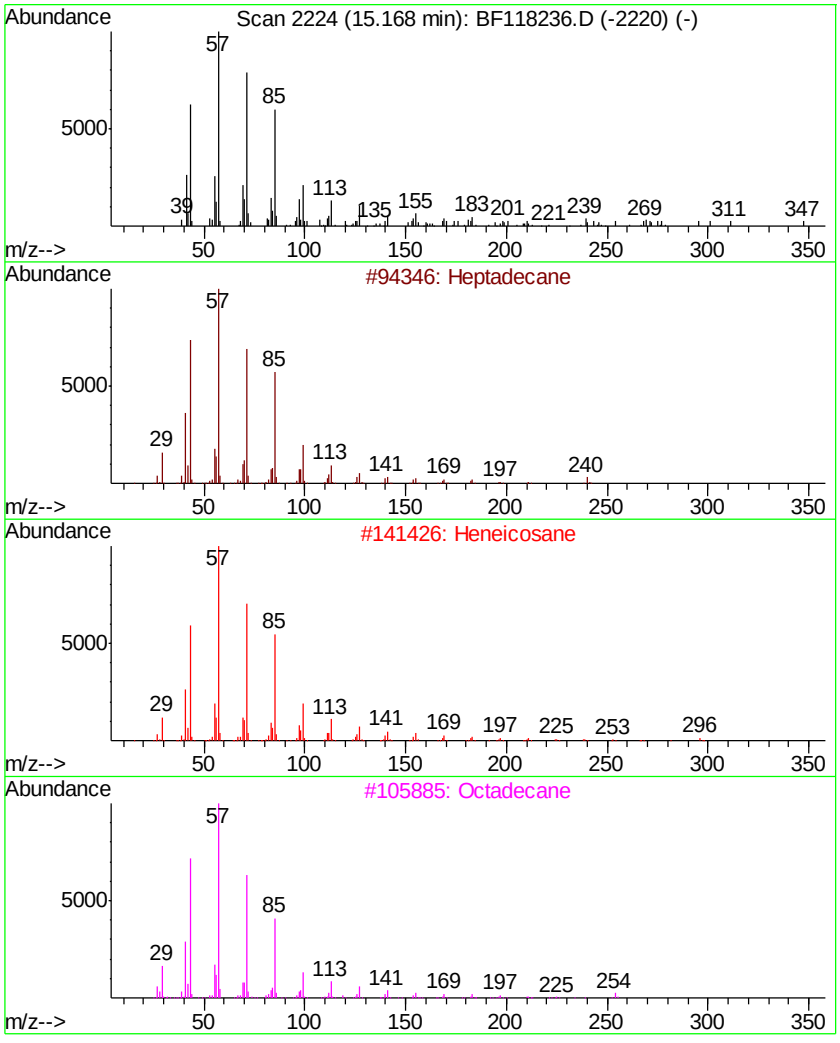
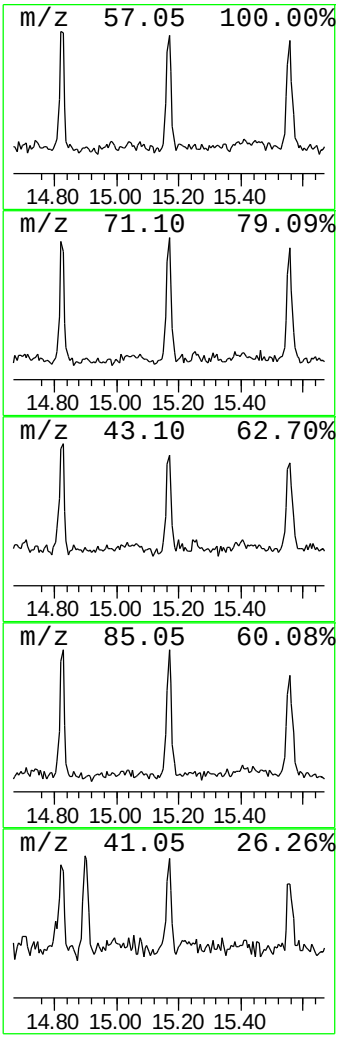
Peak Number 11 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.64 ng	98710	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Docosane	310	C22H46	000629-97-0	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118236.D
Acq On : 17 Dec 2019 19:51
Operator : JU
Sample : K6327-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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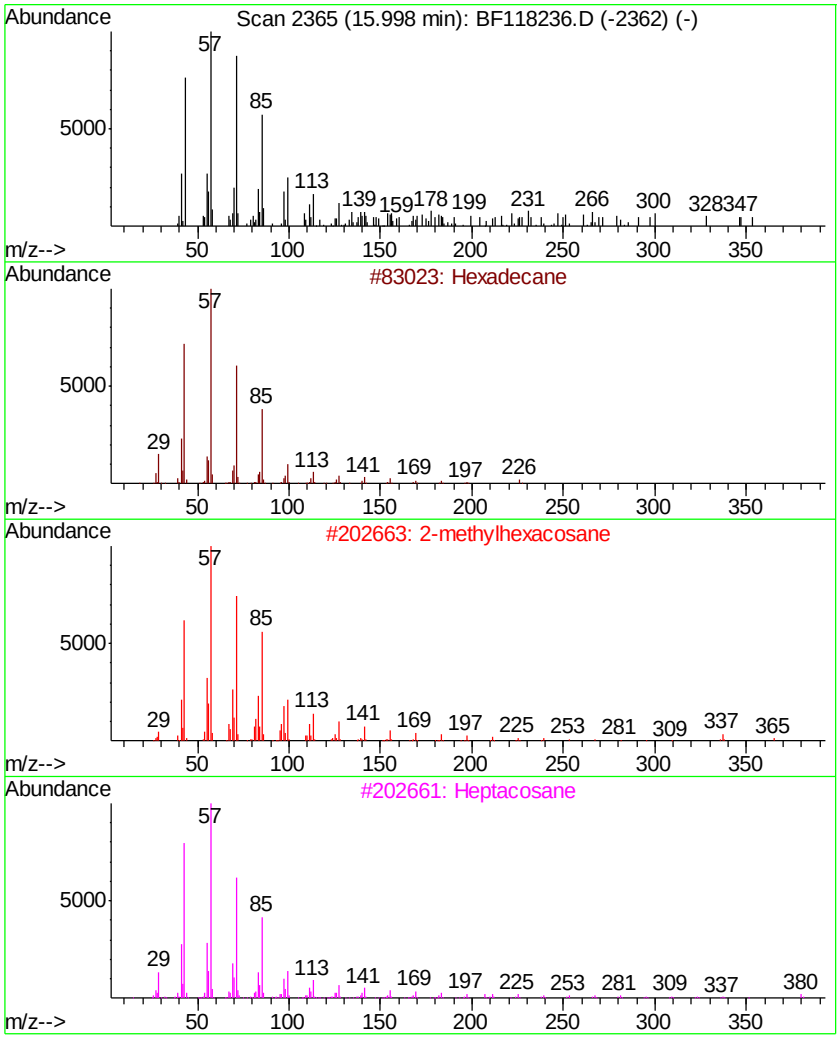
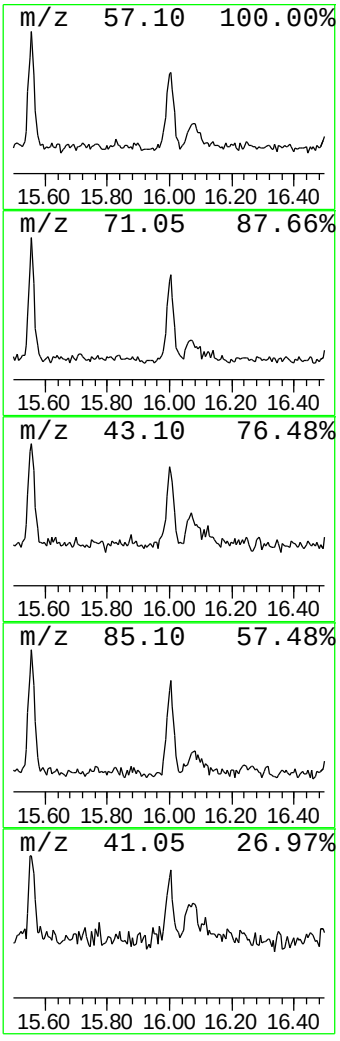
Peak Number 12 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.44 ng	91206	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	2-methylhexacosane	380	C27H56	1000376-72-7	76
3	Heptacosane	380	C27H56	000593-49-7	68
4	2-methyloctacosane	408	C29H60	1000376-72-8	68
5	Hentriacontane	437	C31H64	000630-04-6	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
Data File : BF118236.D
Acq On : 17 Dec 2019 19:51
Operator : JU
Sample : K6327-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	10.7	ng	399802	1	6.86	747071	20.0
2-Pentanone, 4-hy...	5.07	12.8	ng	478976	1	6.86	747071	20.0
unknown6.63	6.63	80.2	ng	2995370	1	6.86	747071	20.0
n-Hexadecanoic acid	11.92	5.2	ng	229930	4	11.40	881275	20.0
Octadecyl trifluo...	13.89	11.8	ng	486985	5	14.06	826387	20.0
Nonadecane, 9-met...	14.21	2.0	ng	82755	5	14.06	826387	20.0
Eicosane	14.52	3.0	ng	126133	5	14.06	826387	20.0
Heneicosane	14.83	3.1	ng	114862	6	15.54	748784	20.0
Squalene	14.90	2.2	ng	81129	6	15.54	748784	20.0
Heptadecane	15.17	2.6	ng	98710	6	15.54	748784	20.0
Hexadecane	16.00	2.4	ng	91206	6	15.54	748784	20.0