LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112551.D
Acq On : 13 Feb 2019 21:01
Operator : JU/SJ
Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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-BF012519.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	5.057	501	505	519	rVB	80208	113377	4.60%	0.537%
2	5.475	572	576	592	rBV	2110582	2191282	88.96%	10.381%
3	6.492	744	749	766	rBV	2159368	2363692	95.96%	11.197%
4	6.616	766	770	785	rVB	2858408	2463314	100.00%	11.669%
5	6.833	804	807	816	rBV	653352	605434	24.58%	2.868%
6	6.992	830	834	848	rBV	2142019	1841253	74.75%	8.722%
7	7.398	899	903	923	rBV	1318321	1427877	57.97%	6.764%
8	8.116	1022	1025	1045	rBV	692090	743244	30.17%	3.521%
9	9.192	1204	1208	1219	rBV	2849621	2413456	97.98%	11.433%
10	9.586	1271	1275	1283	rBV	142321	139520	5.66%	0.661%
11	9.874	1320	1324	1334	rBV2	806284	750087	30.45%	3.553%
12	10.669	1456	1459	1474	rBV	1322782	1358283	55.14%	6.435%
13	11.368	1574	1578	1589	rBV	679998	677470	27.50%	3.209%
14	11.886	1663	1666	1674	rBV	155641	178512	7.25%	0.846%
15	12.668	1796	1799	1807	rBV5	35613	48237	1.96%	0.229%
16	12.945	1842	1846	1850	rBV	1932939	1817704	73.79%	8.611%
17	13.833	1994	1997	2006	rBV	151503	239586	9.73%	1.135%
18	14.015	2024	2028	2035	rBV	652269	635578	25.80%	3.011%
19	14.151	2049	2051	2054	rBV	57091	51772	2.10%	0.245%
20	14.457	2100	2103	2106	rBV	98345	102360	4.16%	0.485%
21	14.762	2152	2155	2159	rVB	86209	83362	3.38%	0.395%
22	14.833	2165	2167	2171	rVB	85639	81005	3.29%	0.384%
23	15.092	2208	2211	2216	rVB	120300	133764	5.43%	0.634%
24	15.474	2272	2276	2277	rBV	91750	115291	4.68%	0.546%
25	15.498	2277	2280	2291	rVB2	304984	418725	17.00%	1.984%
26	15.903	2346	2349	2354	rVB	84165	115135	4.67%	0.545%

Sum of corrected areas: 21109320

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112551.D
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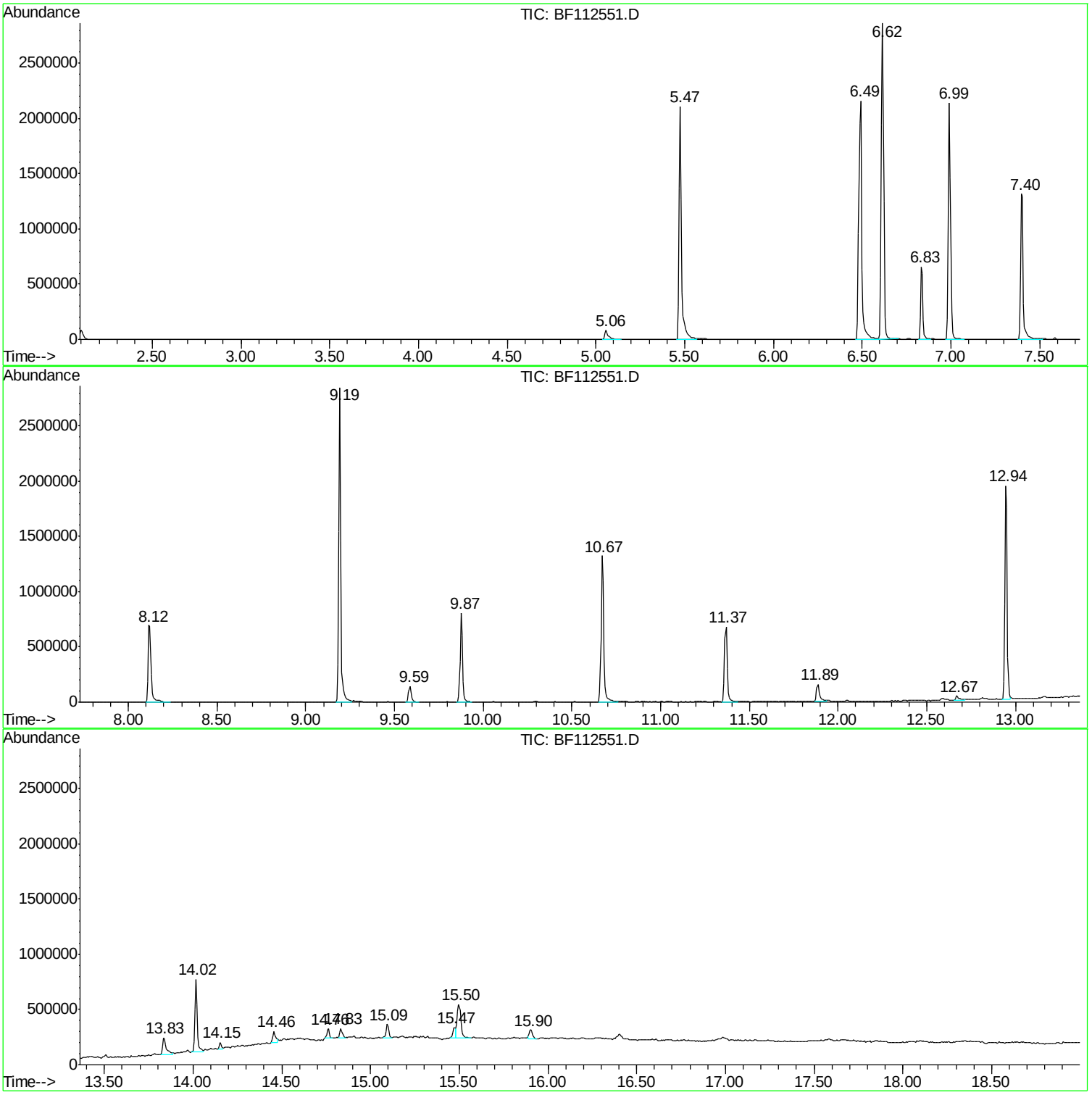
Operator : JU/SJ
Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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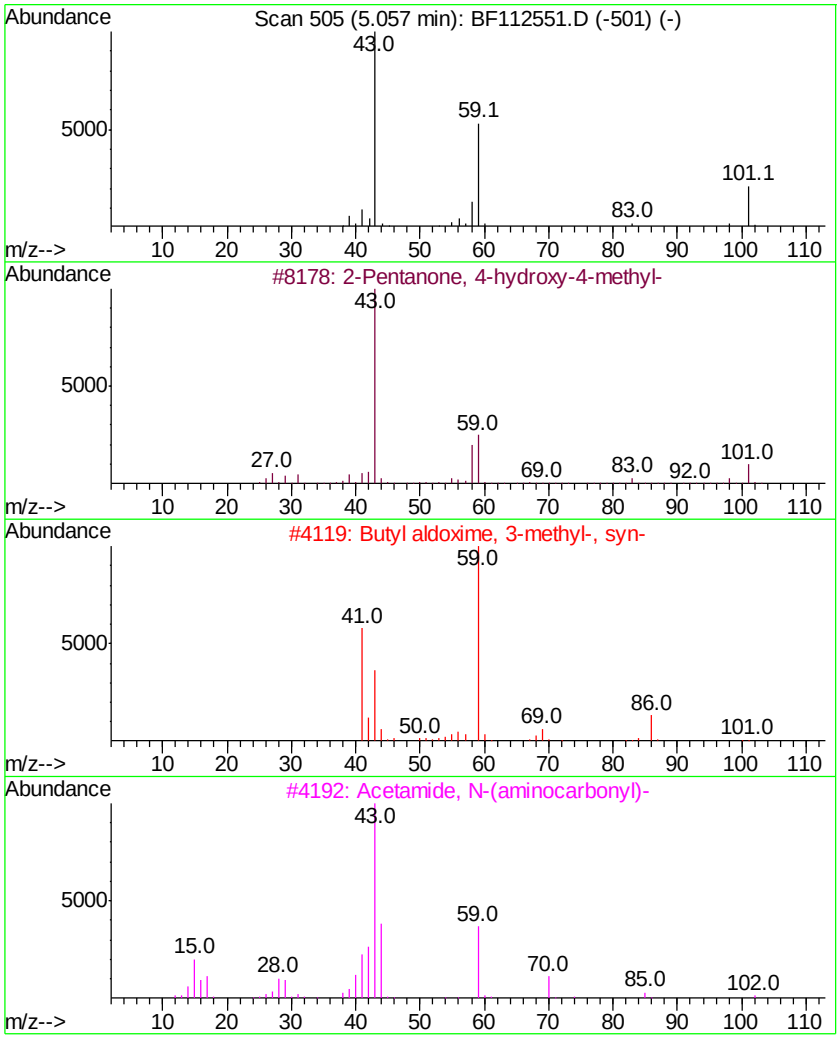
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

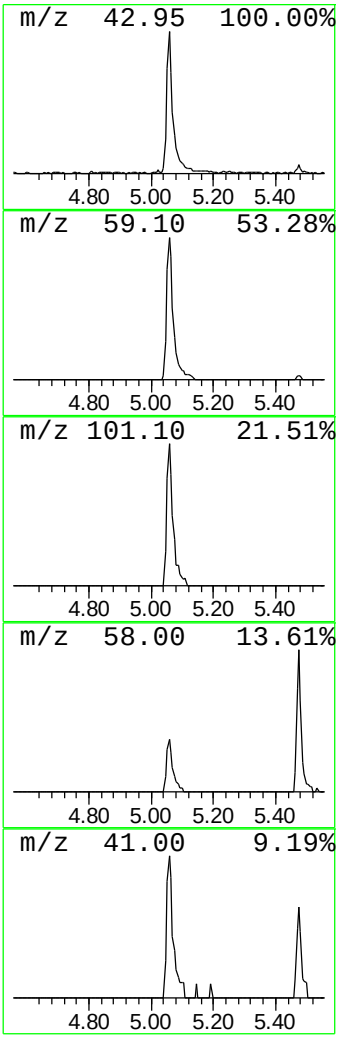
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	3.75 ng	113377	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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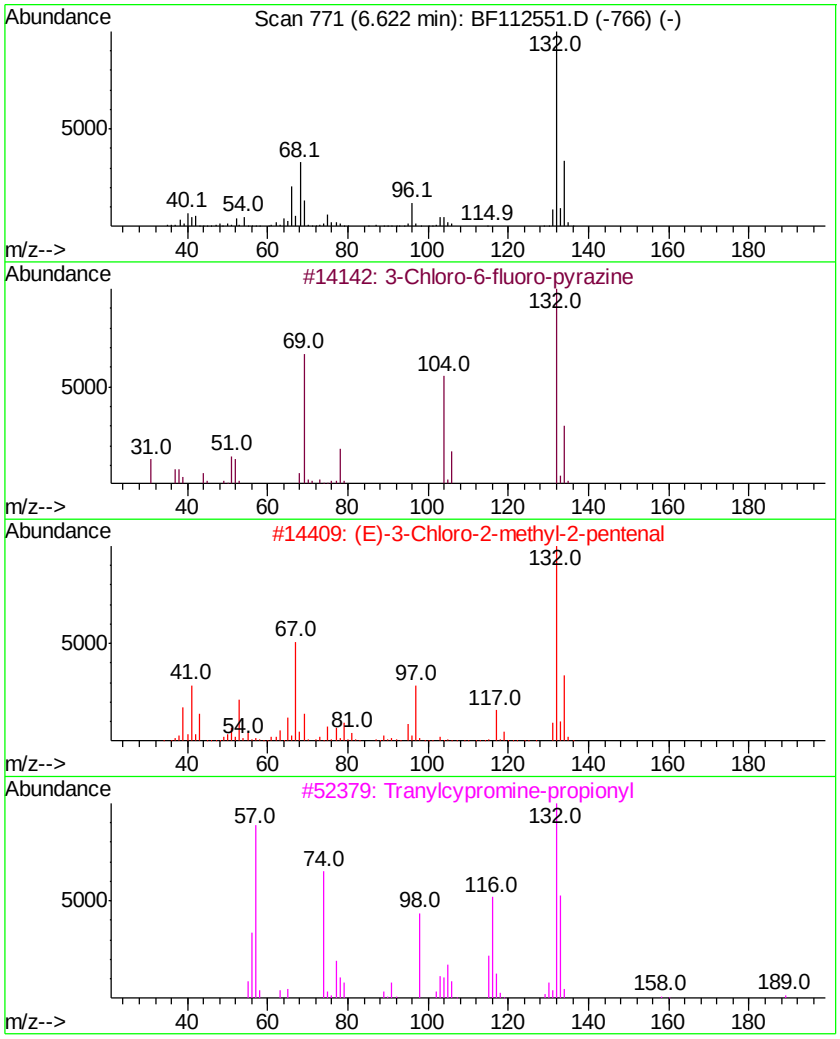
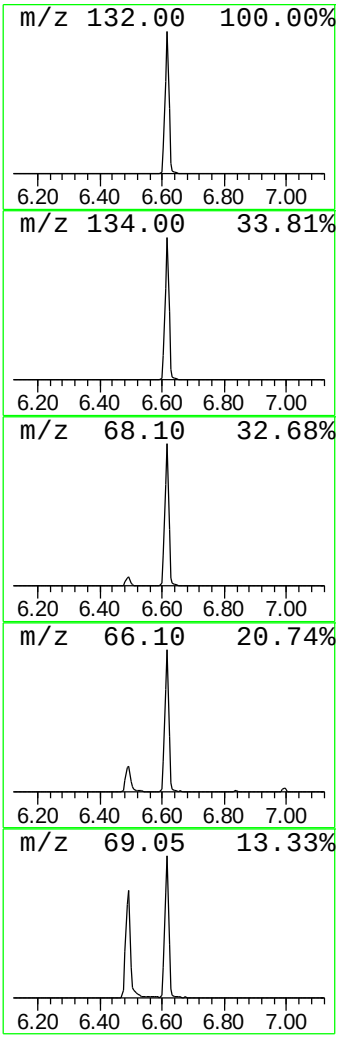
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	81.37 ng	2463310	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112551.D
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Operator : JU/SJ
Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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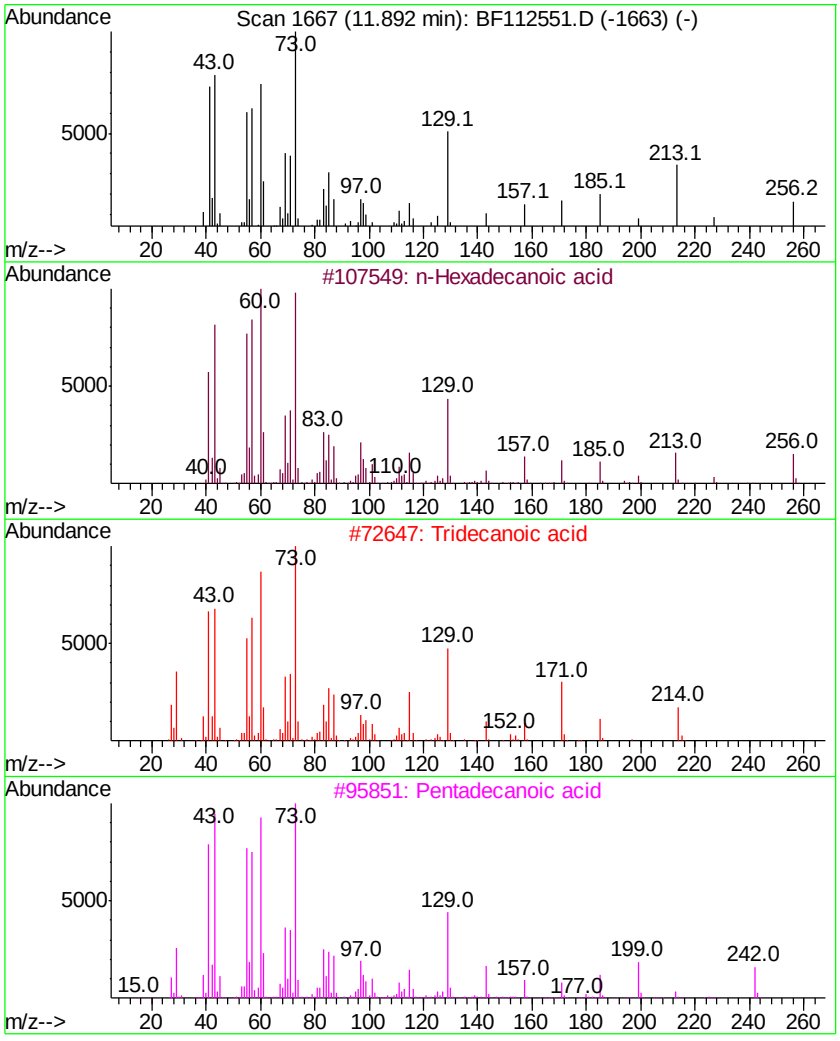
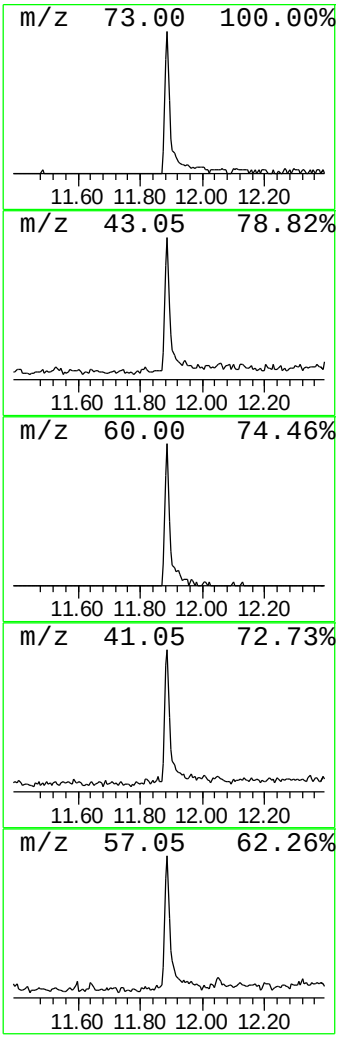
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.27 ng	178512	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

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Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

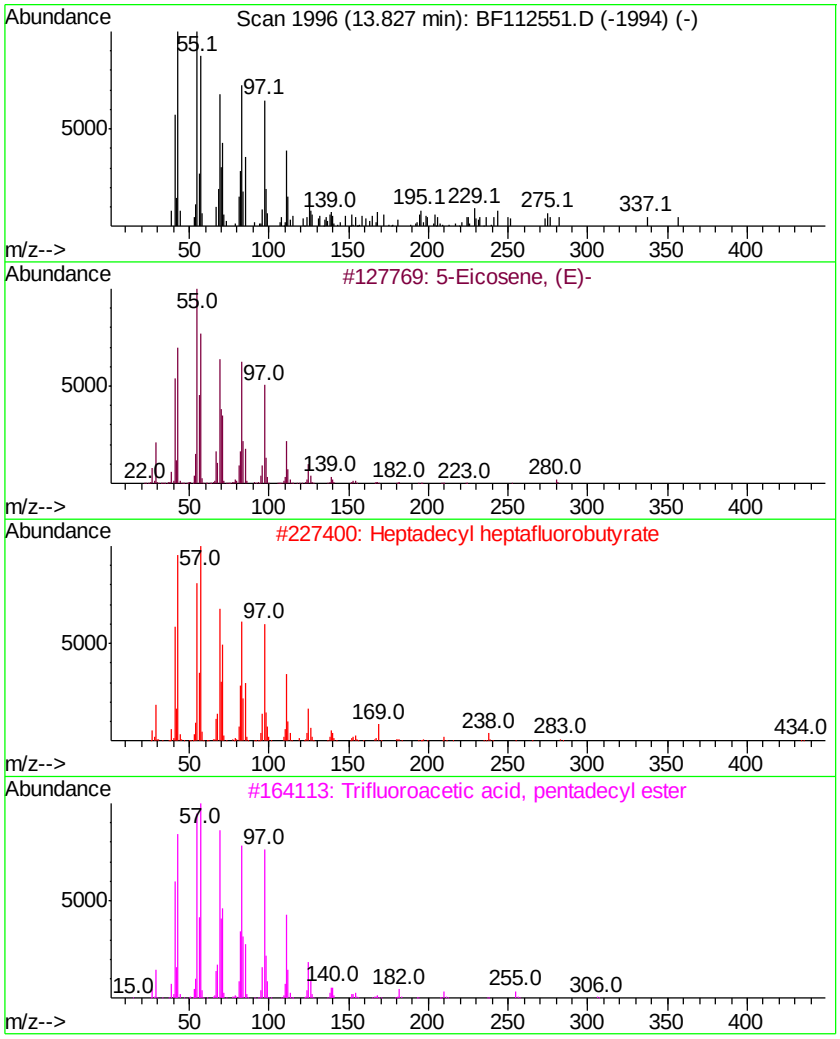
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

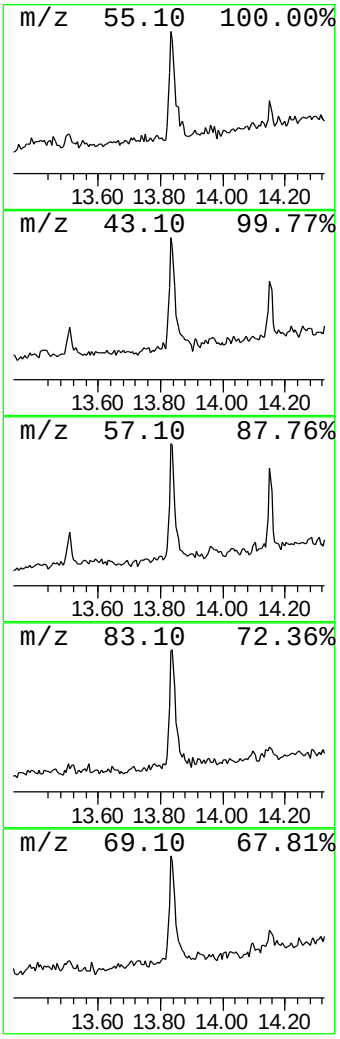
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	7.54 ng	239586	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	1-Tricosene	322	C23H46	018835-32-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
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Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

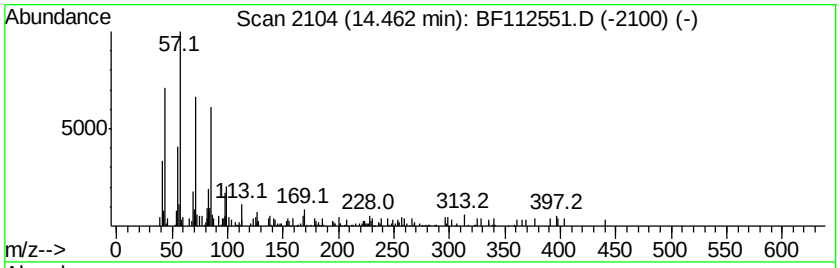
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

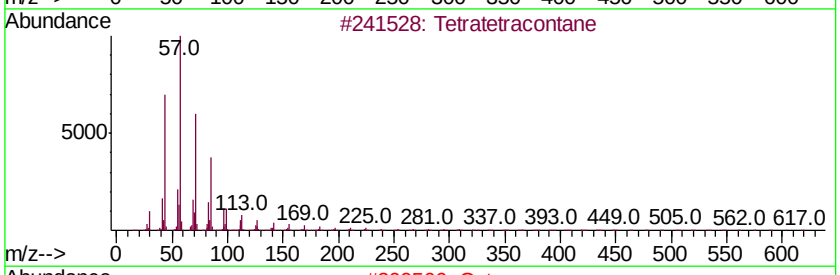
****

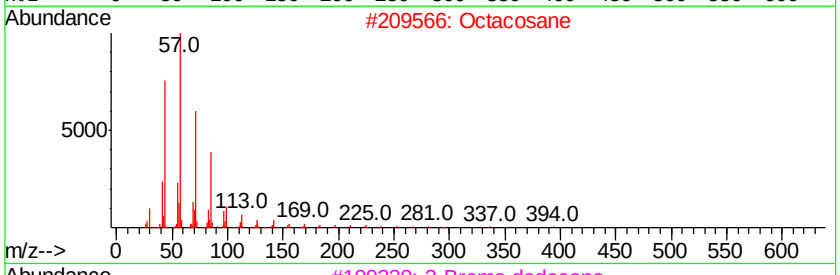
Peak Number 6 Tetratetracontane Concentration Rank 10

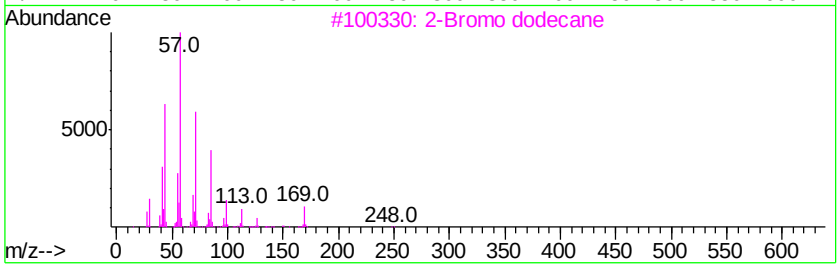
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	3.22 ng	102360	Chrysene-d12	14.02

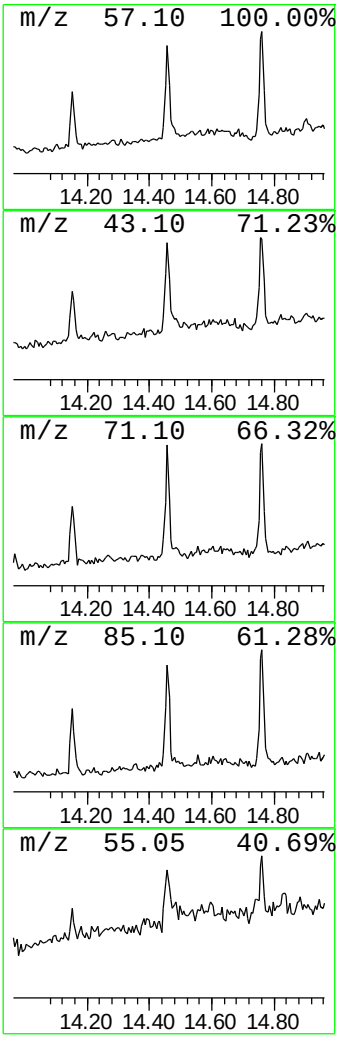
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	87
2	Octacosane	394	C28H58	000630-02-4	86
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Eicosane	282	C20H42	000112-95-8	86











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Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

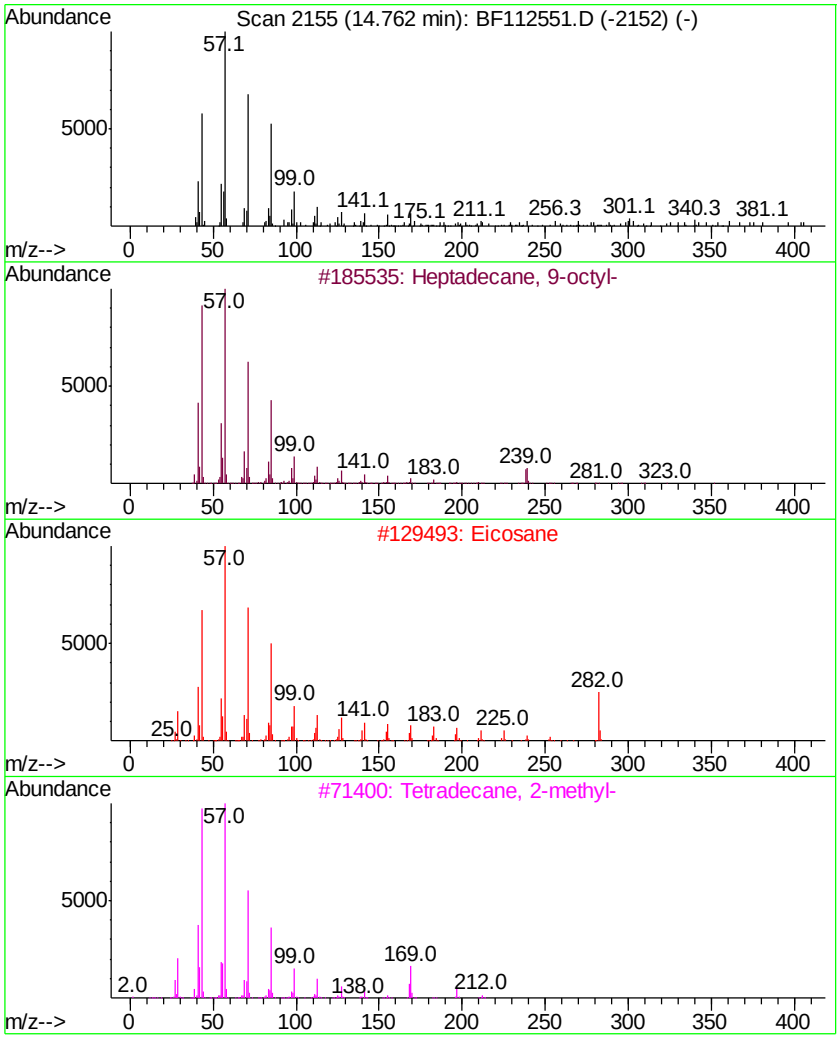
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

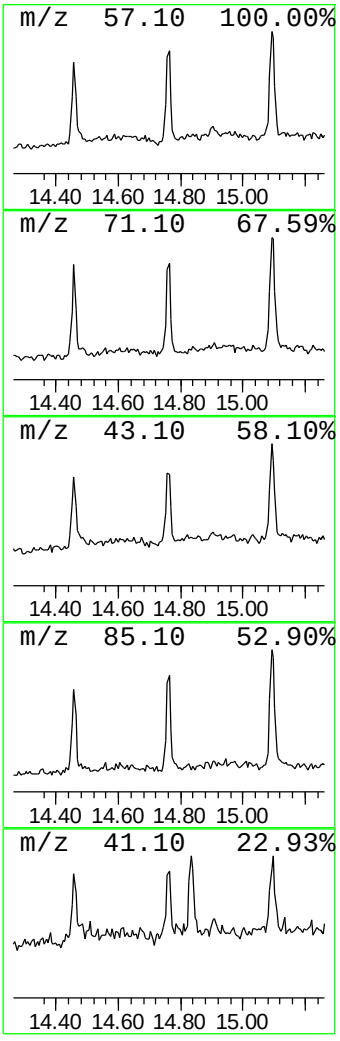
****

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	3.98 ng	83362	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Eicosane	282	C20H42	000112-95-8	87
3	Tetradecane, 2-methyl-	212	C15H32	001560-95-8	87
4	Heneicosane	296	C21H44	000629-94-7	83
5	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	80





Library Search Compound Report

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BNA_F
ClientSampleId :
SB-3

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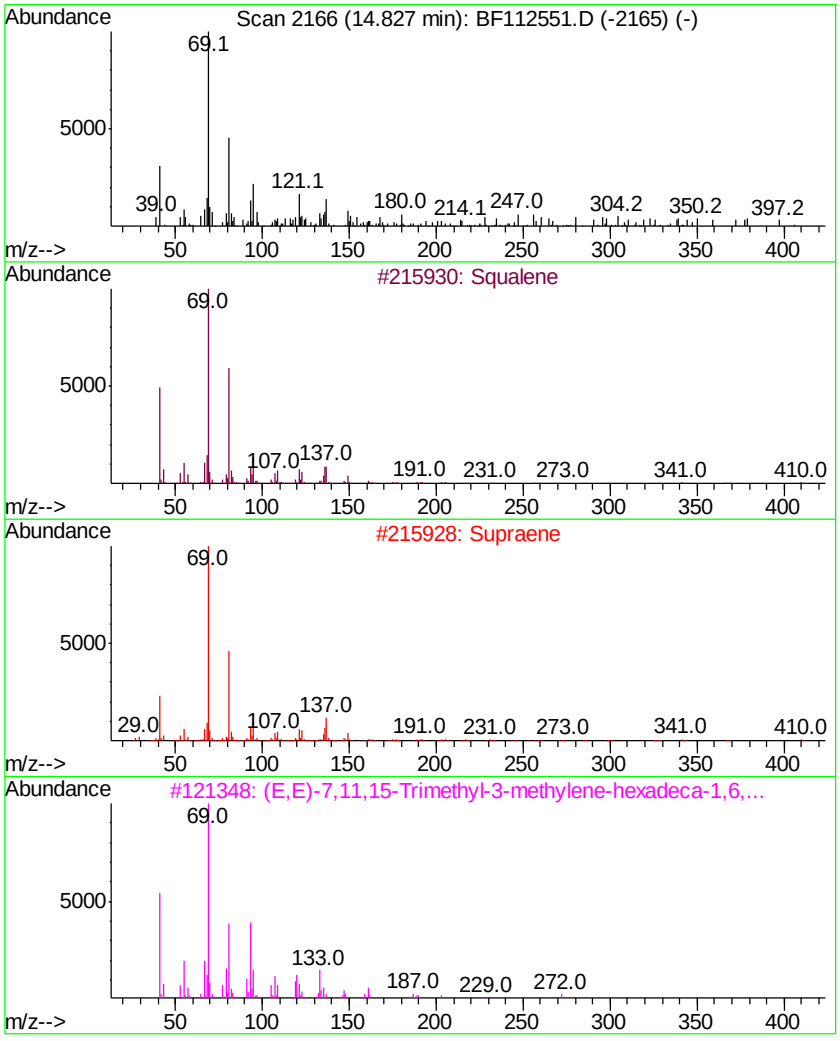
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

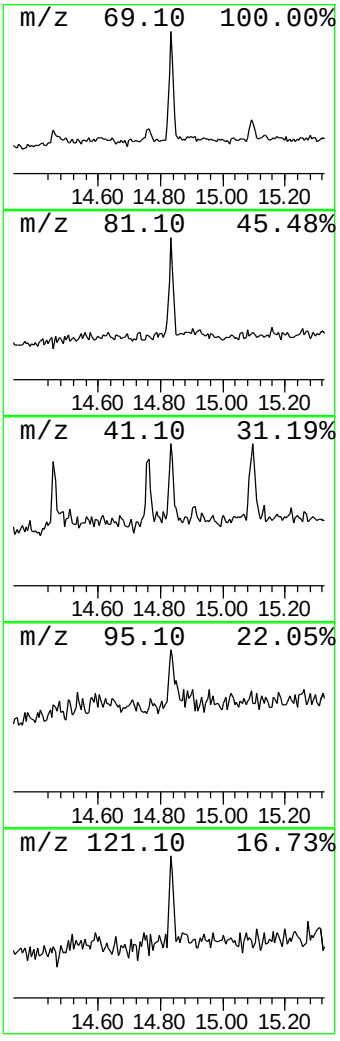
****

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.87 ng	81005	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	83
2	Supraene	410	C30H50	007683-64-9	74
3	(E,E)-7,11,15-Trimethyl-3-methyl...	272	C20H32	070901-63-2	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
5	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	53





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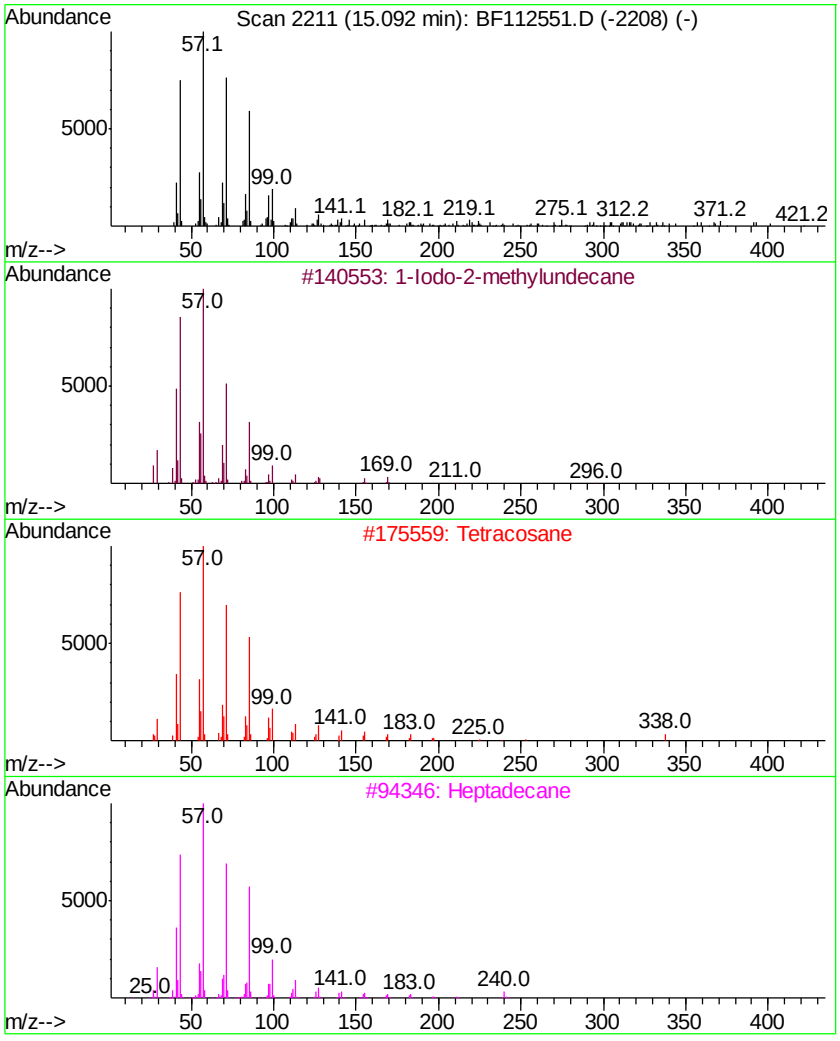
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

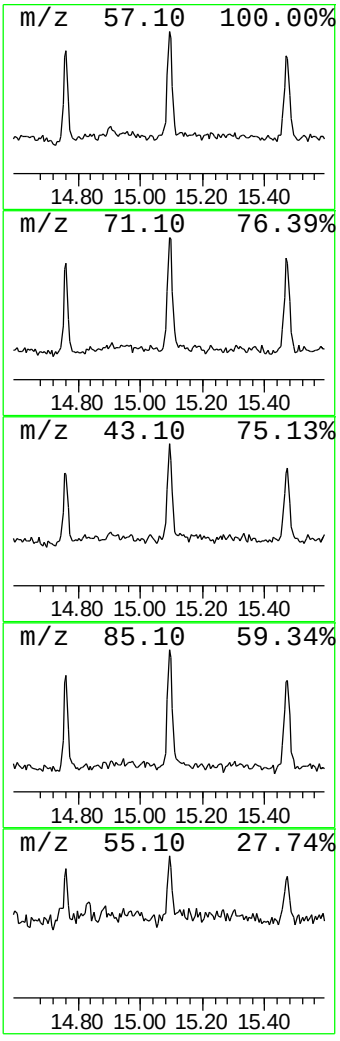
****

Peak Number 9 1-Iodo-2-methylundecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	6.39 ng	133764	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Hexadecane	226	C16H34	000544-76-3	81
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	80





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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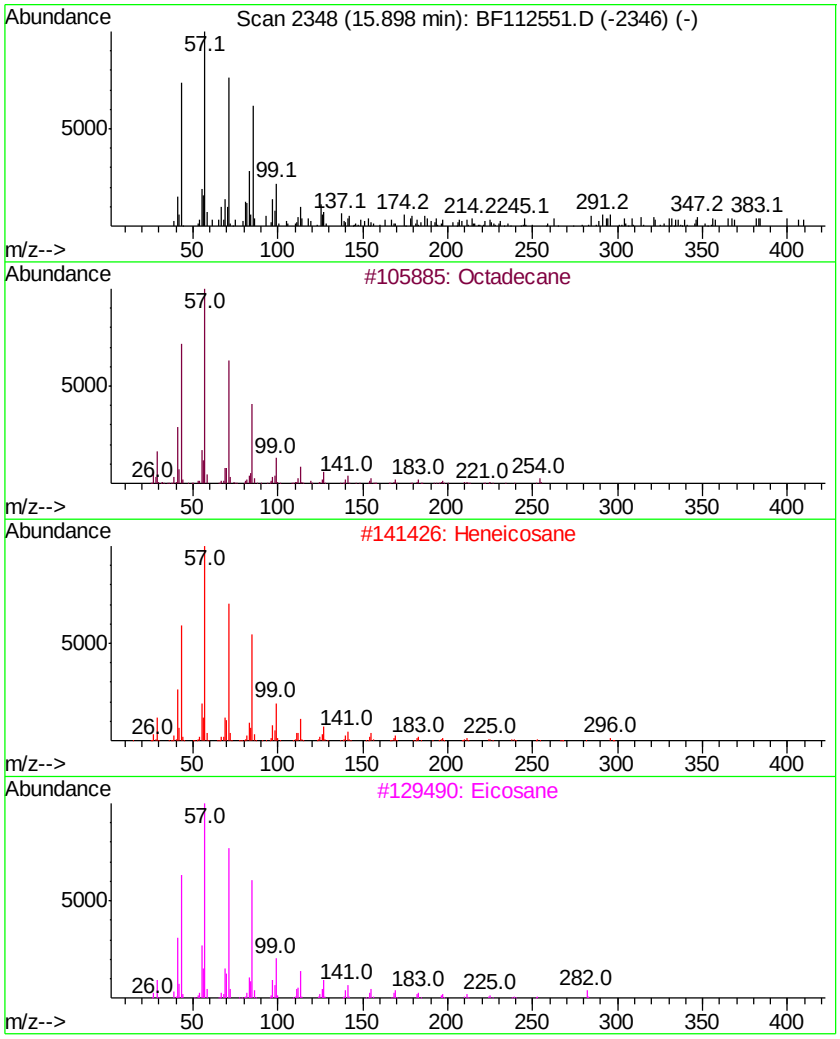
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

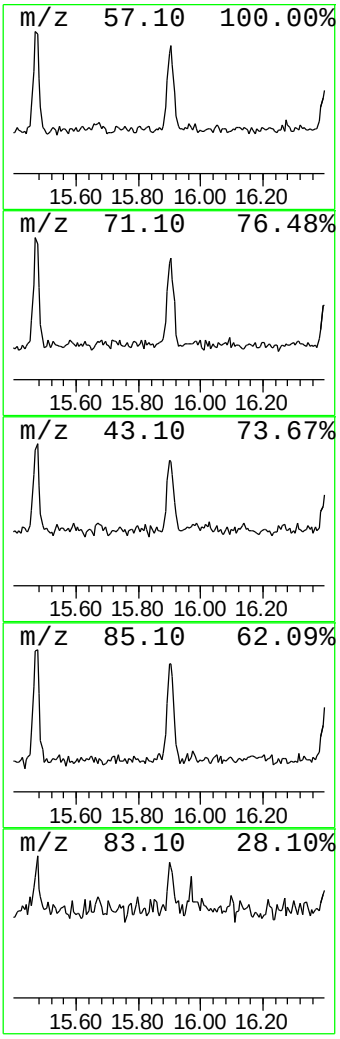
****

Peak Number 10 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	5.50 ng	115135	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Heneicosane	296	C21H44	000629-94-7	68
3	Eicosane	282	C20H42	000112-95-8	68
4	Tetracosane	338	C24H50	000646-31-1	68
5	Tridecane	184	C13H28	000629-50-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112551.D
Acq On : 13 Feb 2019 21:01
Operator : JU/SJ
Sample : K1458-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
2-Pentanone, 4-hy...	5.06	3.8	ng	113377	1	6.83	605434	20.0
unknown6.62	6.62	81.4	ng	2463310	1	6.83	605434	20.0
n-Hexadecanoic acid	11.89	5.3	ng	178512	4	11.37	677470	20.0
5-Eicosene, (E)-	13.83	7.5	ng	239586	5	14.02	635578	20.0
Tetratetracontane	14.46	3.2	ng	102360	5	14.02	635578	20.0
Heptadecane, 9-oc...	14.76	4.0	ng	83362	6	15.50	418725	20.0
Squalene	14.83	3.9	ng	81005	6	15.50	418725	20.0
1-Iodo-2-methylun...	15.09	6.4	ng	133764	6	15.50	418725	20.0
Octadecane	15.90	5.5	ng	115135	6	15.50	418725	20.0