LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108044.D
Acq On : 9 Aug 2018 11:24
Operator : JU/SJ
Sample : J4275-03 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-080718-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-BF080818.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	5.231	489	492	498	rVB	187893	177698	6.37%	0.758%
2	5.619	554	558	562	rBV	1127349	961776	34.48%	4.102%
3	6.613	723	727	730	rBV	1371004	1063691	38.13%	4.537%
4	6.772	751	754	758	rBV	1154953	1039205	37.26%	4.432%
5	7.013	791	795	798	rBV	2290367	1859649	66.67%	7.932%
6	7.166	817	821	825	rVB	1005581	814597	29.20%	3.474%
7	7.566	886	889	893	rBV	848320	658582	23.61%	2.809%
8	8.295	1009	1013	1017	rBV	3016299	2484439	89.07%	10.596%
9	8.578	1056	1061	1066	rVB7	31515	51090	1.83%	0.218%
10	9.307	1182	1185	1187	rVB	47418	41486	1.49%	0.177%
11	9.372	1191	1196	1199	rBV	1501178	1293282	46.36%	5.516%
12	9.442	1205	1208	1211	rBV2	40296	49161	1.76%	0.210%
13	9.760	1259	1262	1266	rBV	156916	132472	4.75%	0.565%
14	9.919	1285	1289	1292	rBV5	26848	32481	1.16%	0.139%
15	9.972	1295	1298	1302	rVB	50444	46927	1.68%	0.200%
16	10.060	1309	1313	1317	rBV	3340305	2789355	100.00%	11.897%
17	10.466	1378	1382	1386	rVB5	33621	50435	1.81%	0.215%
18	10.848	1443	1447	1457	rBV	725842	646446	23.18%	2.757%
19	10.960	1462	1466	1470	rVB3	34376	54816	1.97%	0.234%
20	11.430	1543	1546	1549	rBV	41294	36168	1.30%	0.154%
21	11.554	1563	1567	1571	rBV	3099667	2739249	98.20%	11.683%
22	11.901	1621	1626	1629	rVB	70767	91124	3.27%	0.389%
23	12.060	1649	1653	1656	rBV2	111337	116952	4.19%	0.499%
24	12.101	1657	1660	1664	rVB	65357	79200	2.84%	0.338%
25	12.771	1771	1774	1778	rBV	103966	87337	3.13%	0.373%
26	12.848	1784	1787	1795	rBV7	50726	85284	3.06%	0.364%
27	13.007	1811	1814	1820	rVB	105653	116204	4.17%	0.496%
28	13.142	1833	1837	1840	rBV	1256970	1085339	38.91%	4.629%
29	14.207	2014	2018	2022	rBV	2283195	2102949	75.39%	8.969%
30	15.360	2211	2214	2220	rVB	226495	252986	9.07%	1.079%
31	15.771	2279	2284	2293	rVB	1569181	2078570	74.52%	8.865%
32	16.259	2363	2367	2372	rVB	214430	326939	11.72%	1.394%

LSC Area Percent Report

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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 23445889

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108044.D
Acq On : 9 Aug 2018 11:24
Operator : JU/SJ
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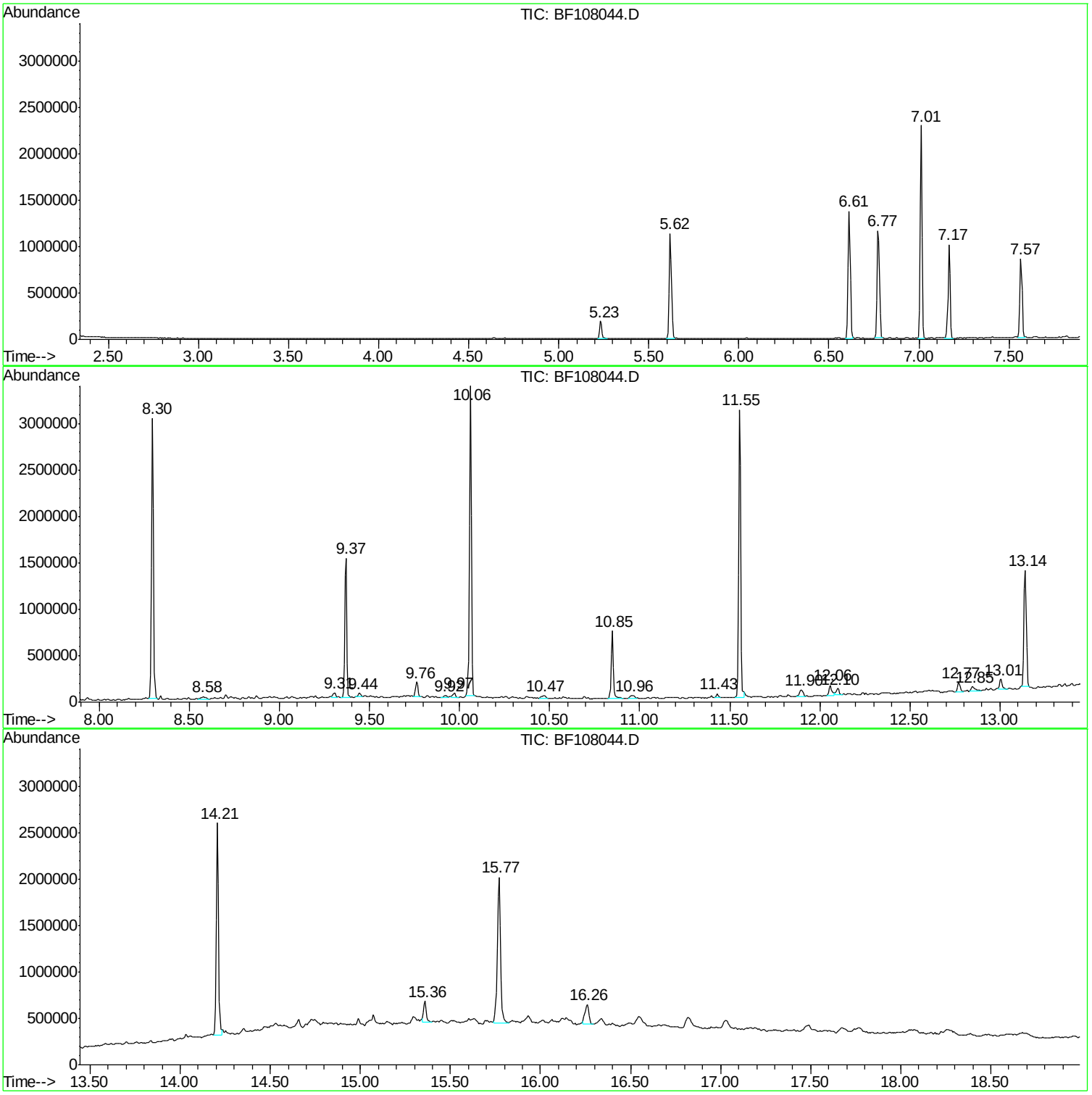
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-080718-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108044.D
Acq On : 9 Aug 2018 11:24
Operator : JU/SJ
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-080718-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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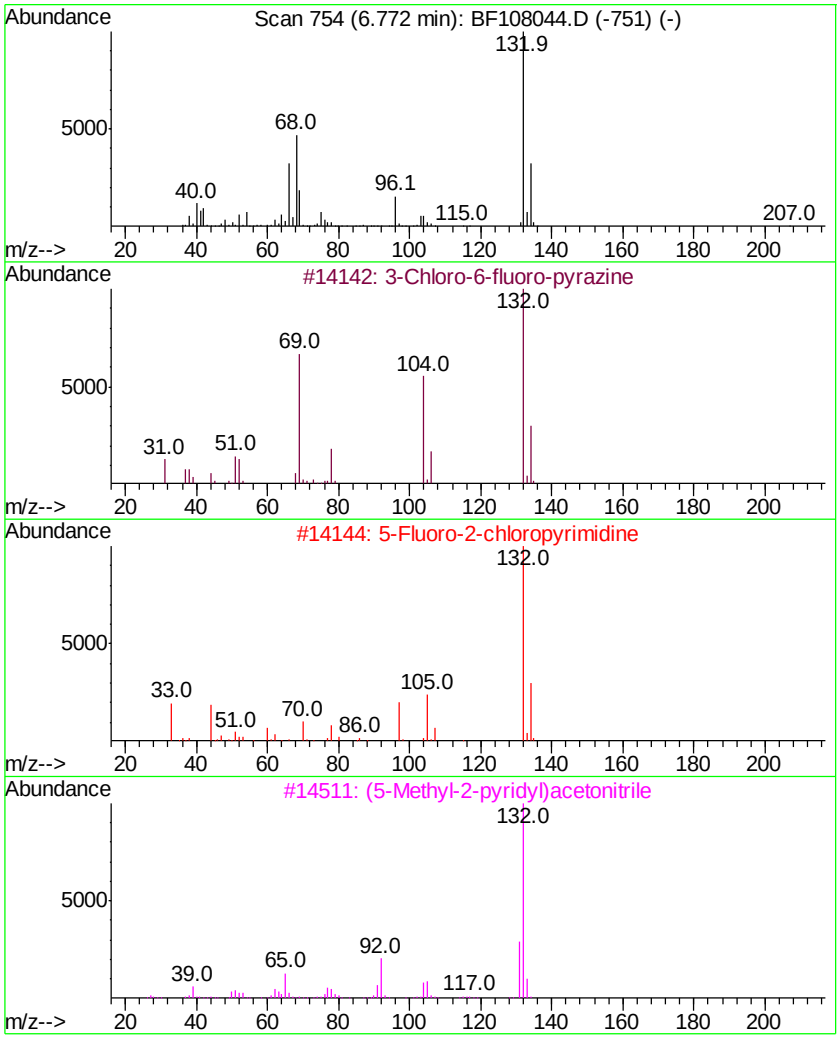
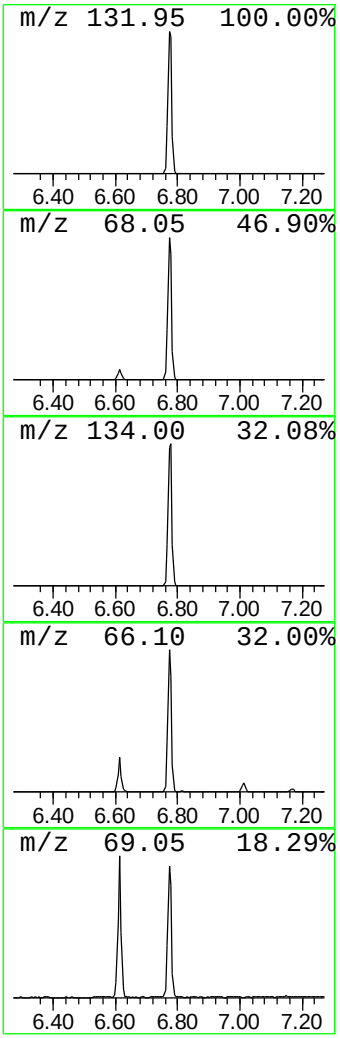
Peak Number 1 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	11.18 ng	1039210	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Instrument : BNA_F
ClientSampleId : CL-02-080718-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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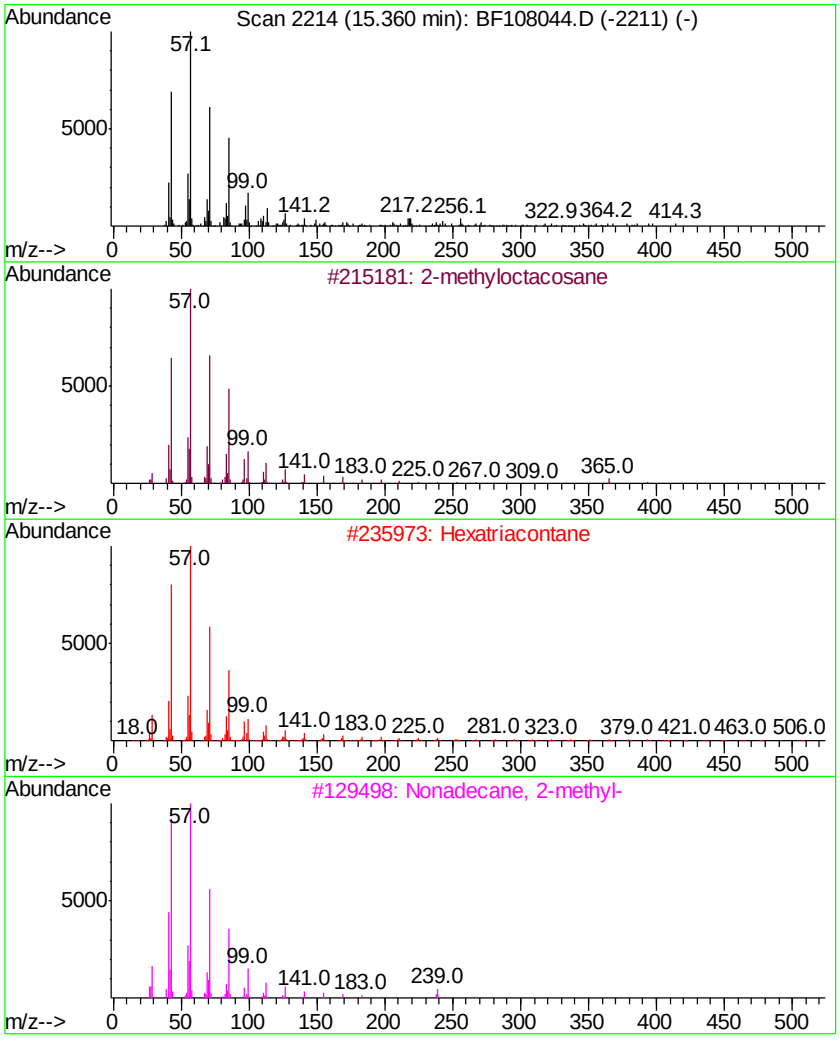
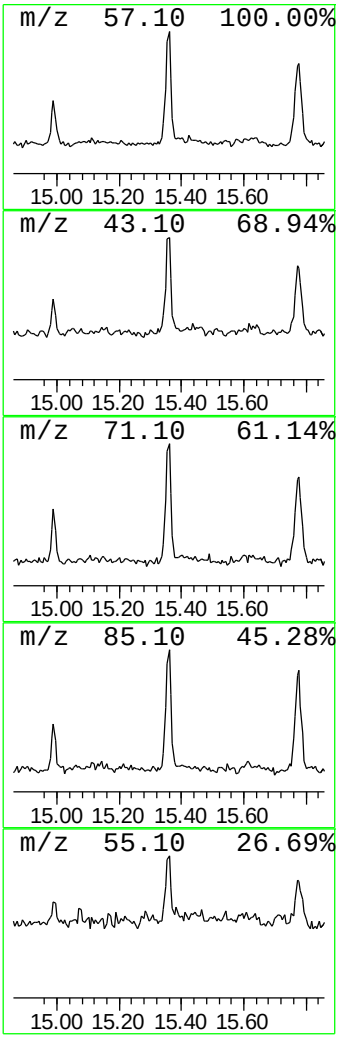
Peak Number 3 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.43 ng	252986	Perylene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Hexatriacontane	507	C36H74	000630-06-8	87
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





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Sample : J4275-03 5X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-080718-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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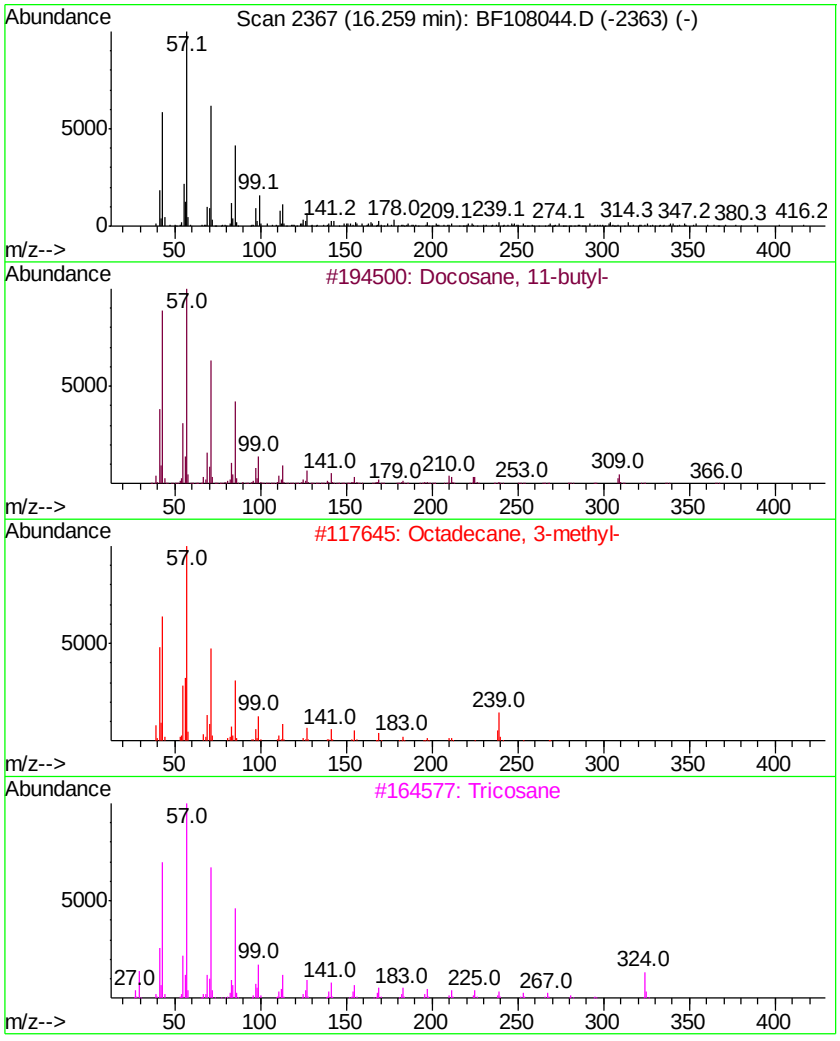
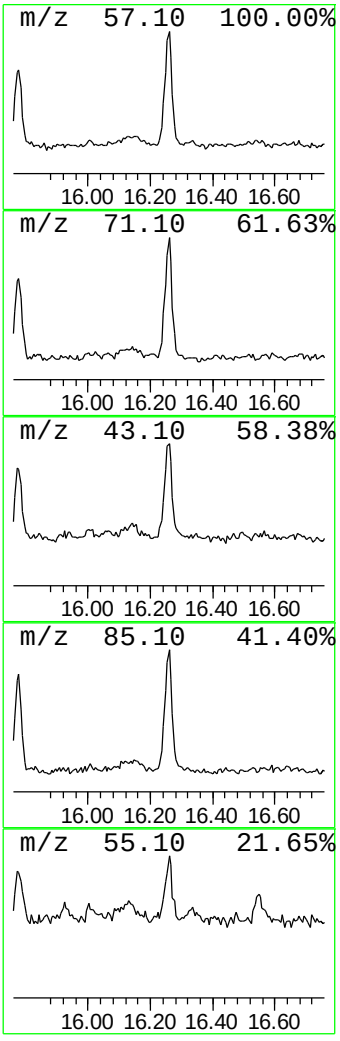
Peak Number 4 Docosane, 11-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.26	3.15 ng	326939	Perylene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2	Octadecane, 3-methyl-	268	C19H40	006561-44-0	87
3	Tricosane	324	C23H48	000638-67-5	87
4	Hexadecane, 6,11-dipentyl-	366	C26H54	015874-03-0	87
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.77	6.77	11.2	ng	1039210	1	7.01	1859650	20.0
2-methyloctacosane	15.36	2.4	ng	252986	6	15.77	2078570	20.0
Docosane, 11-butyl-	16.26	3.1	ng	326939	6	15.77	2078570	20.0