LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103240.D
Acq On : 27 Feb 2018 1:29
Operator : SJ/JU
Sample : J1660-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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	2.163	5	13	20	rVB	1019695	1422121	36.61%	4.311%
2	5.116	511	515	527	rVB	142427	201685	5.19%	0.611%
3	5.504	576	581	599	rBV	3727767	3884538	100.00%	11.777%
4	6.516	747	753	771	rBV	3189622	3790267	97.57%	11.491%
5	6.651	771	776	779	rBV	3544985	3625863	93.34%	10.992%
6	6.875	810	814	820	rBV	1125153	904263	23.28%	2.741%
7	7.034	836	841	844	rBV	3070854	2844762	73.23%	8.624%
8	7.440	905	910	913	rBV	2322622	2269398	58.42%	6.880%
9	8.157	1028	1032	1050	rBV	1271087	1169605	30.11%	3.546%
10	9.234	1210	1215	1218	rBV	3577042	3412279	87.84%	10.345%
11	9.622	1276	1281	1289	rBV	231835	225318	5.80%	0.683%
12	9.833	1313	1317	1321	rBV	97294	84109	2.17%	0.255%
13	9.916	1327	1331	1345	rVB	1193259	1089160	28.04%	3.302%
14	10.333	1398	1402	1404	rVB	84325	74029	1.91%	0.224%
15	10.710	1461	1466	1479	rBV	1730257	1798757	46.31%	5.453%
16	10.804	1479	1482	1492	rVB	55982	60310	1.55%	0.183%
17	11.404	1581	1584	1592	rBV	953067	937362	24.13%	2.842%
18	11.916	1668	1671	1680	rBV4	28276	45043	1.16%	0.137%
19	12.798	1817	1821	1824	rBV	246308	216401	5.57%	0.656%
20	12.851	1826	1830	1832	rVV2	49071	56301	1.45%	0.171%
21	12.874	1832	1834	1839	rVB	76828	63685	1.64%	0.193%
22	12.992	1849	1854	1857	rBV	2615037	2574234	66.27%	7.804%
23	13.504	1937	1941	1944	rBV	215576	183187	4.72%	0.555%
24	13.545	1945	1948	1950	rBV2	50413	47069	1.21%	0.143%
25	13.874	2000	2004	2013	rBV	312206	396819	10.22%	1.203%
26	14.057	2031	2035	2042	rVB	699789	734408	18.91%	2.226%
27	14.192	2056	2058	2061	rBV	56994	56553	1.46%	0.171%
28	14.504	2109	2111	2117	rBV2	66374	62261	1.60%	0.189%
29	14.816	2161	2164	2169	rVB	78293	79863	2.06%	0.242%
30	15.557	2285	2290	2303	rVB	427357	675711	17.39%	2.049%

Sum of corrected areas: 32985361

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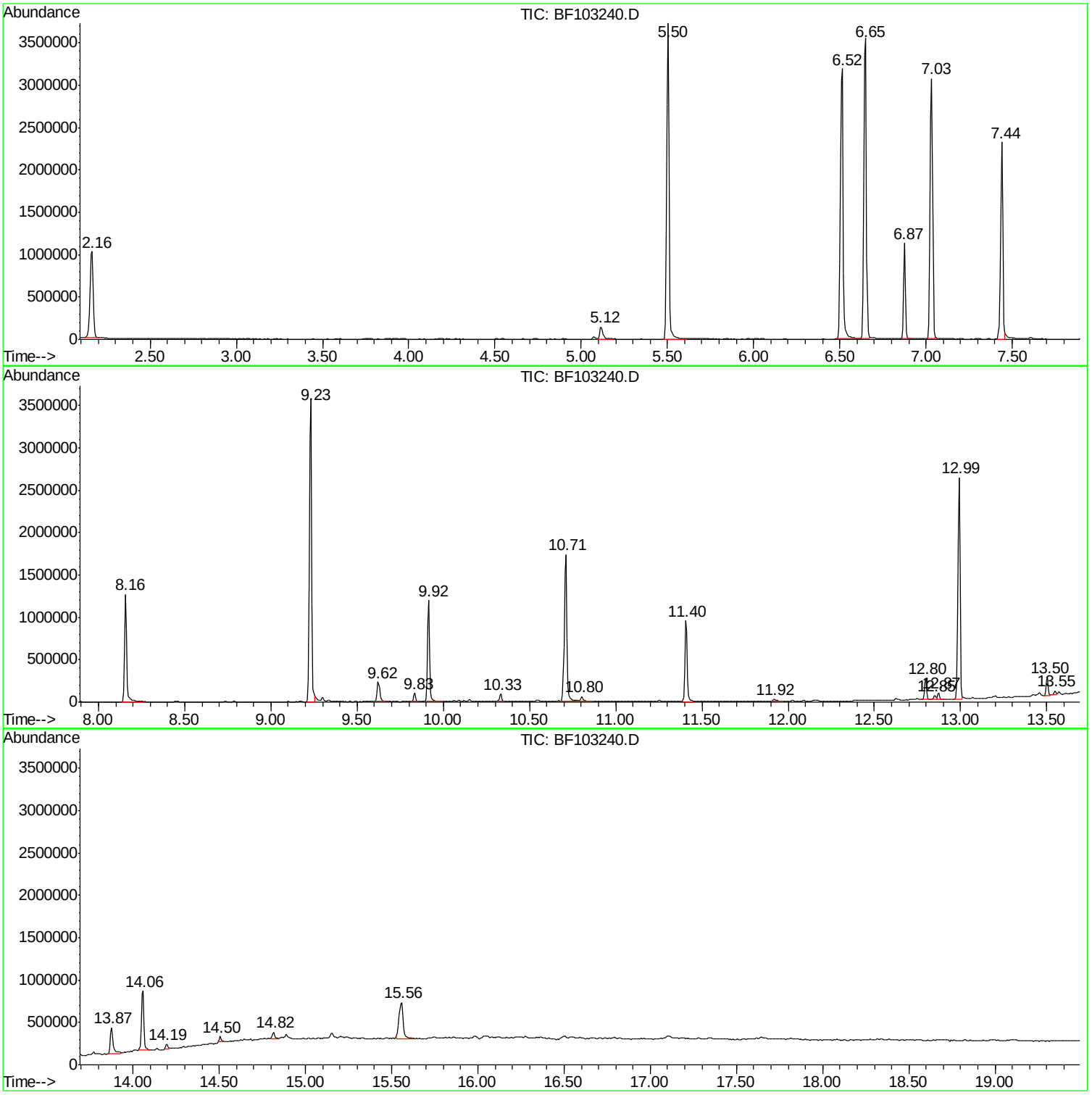
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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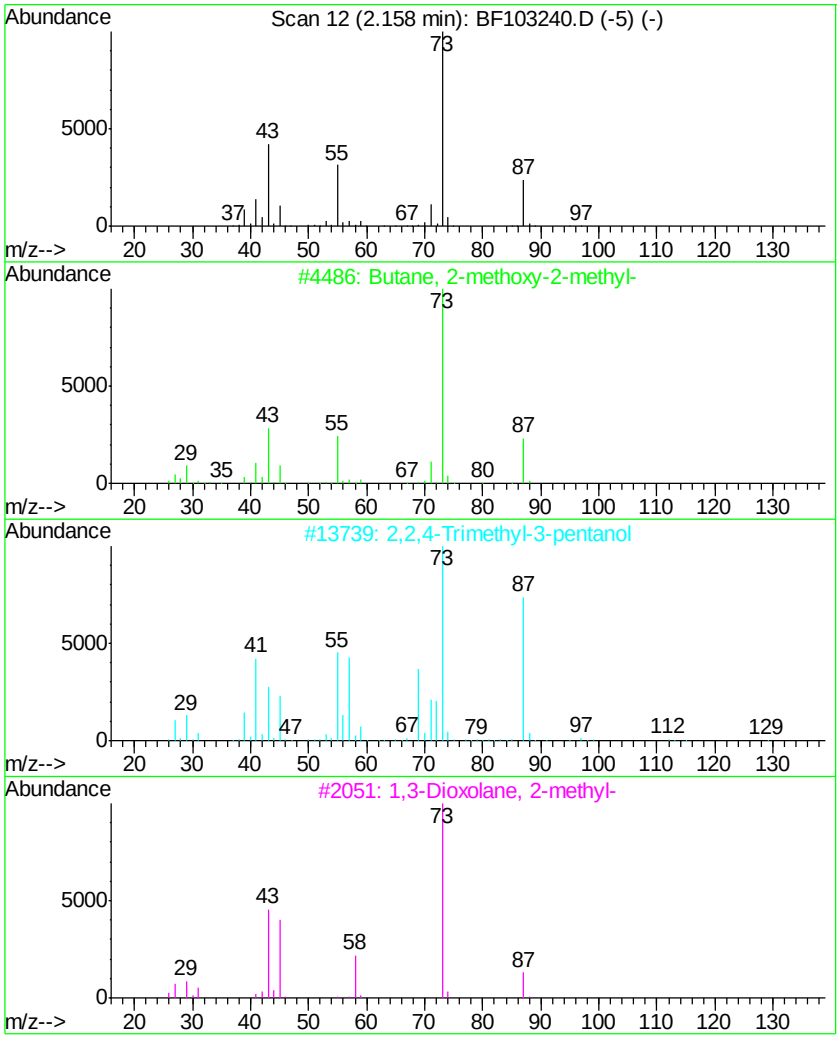
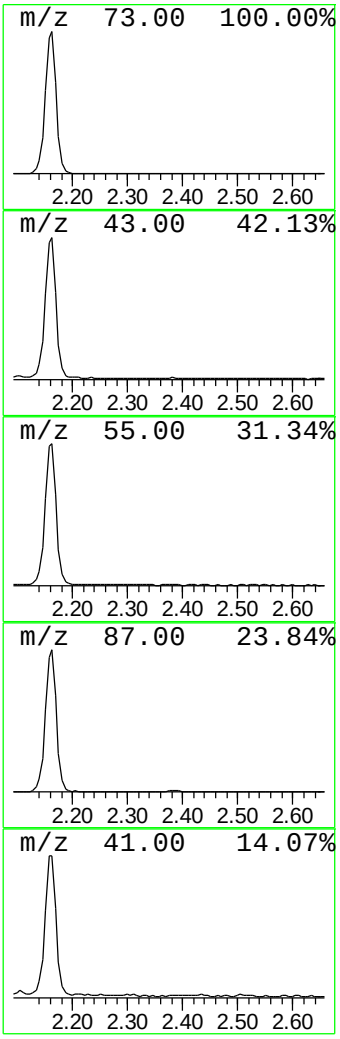
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	31.45 ng	1422120	1,4-Dichlorobenzene-d4	6.87

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Sample : J1660-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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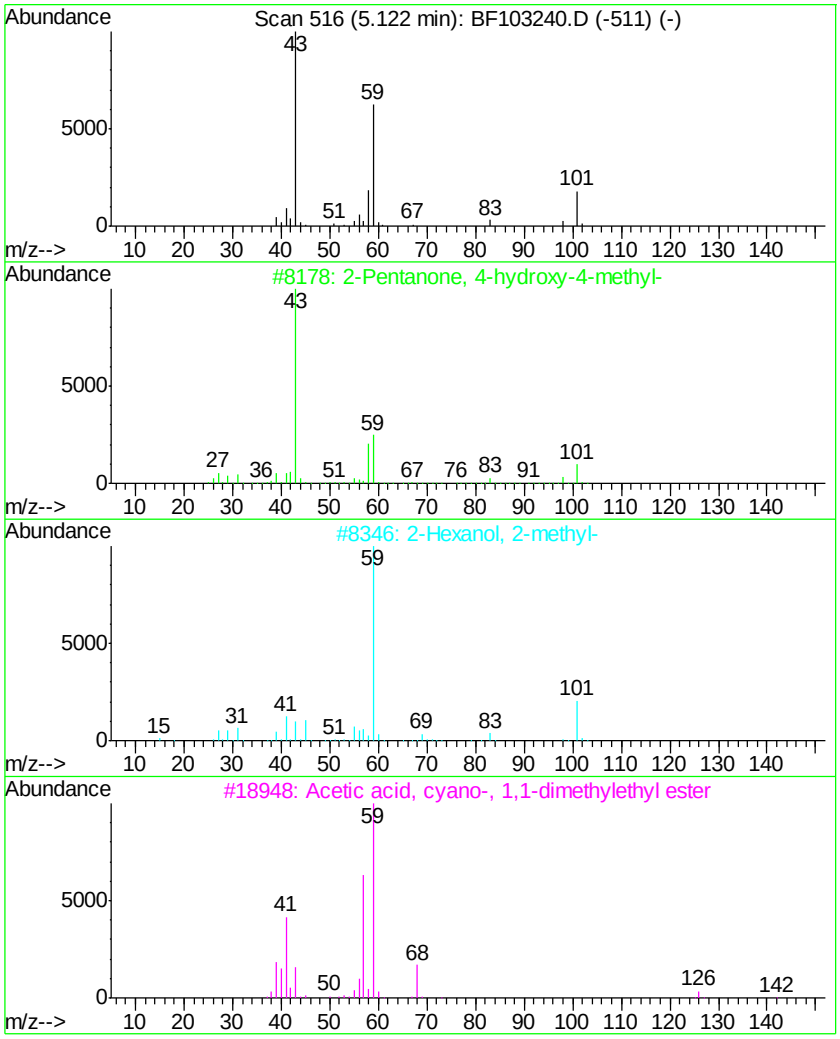
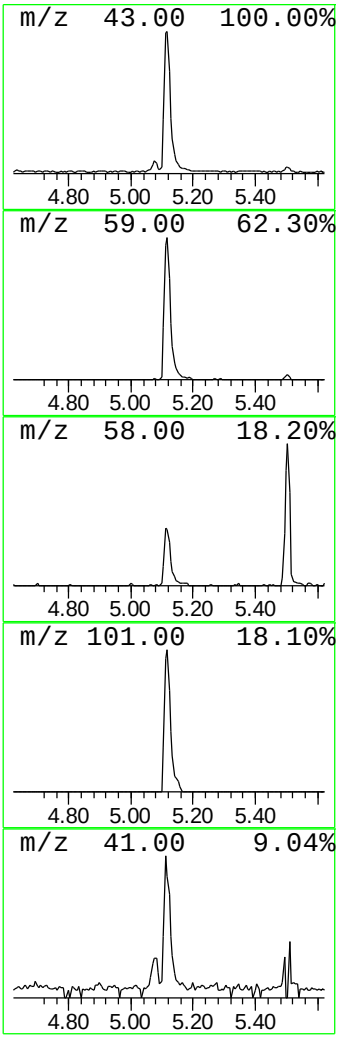
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.46 ng	201685	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Guanidine	59	CH5N3	000113-00-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103240.D
Acq On : 27 Feb 2018 1:29
Operator : SJ/JU
Sample : J1660-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

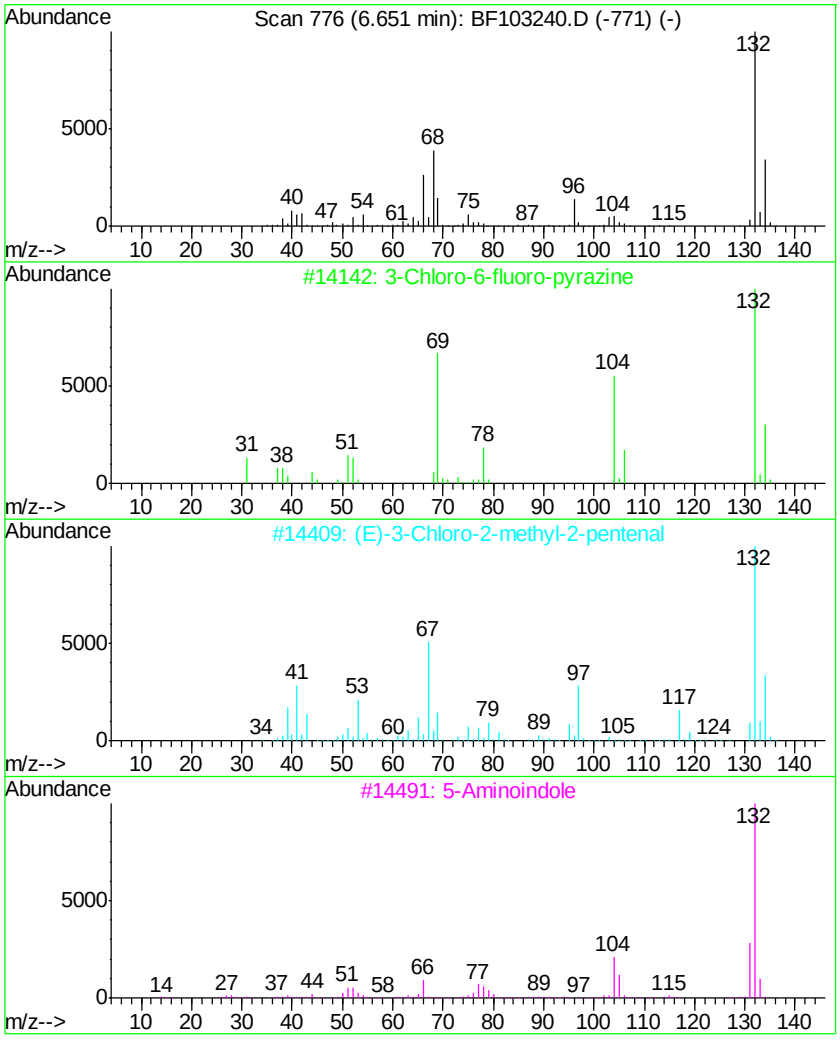
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

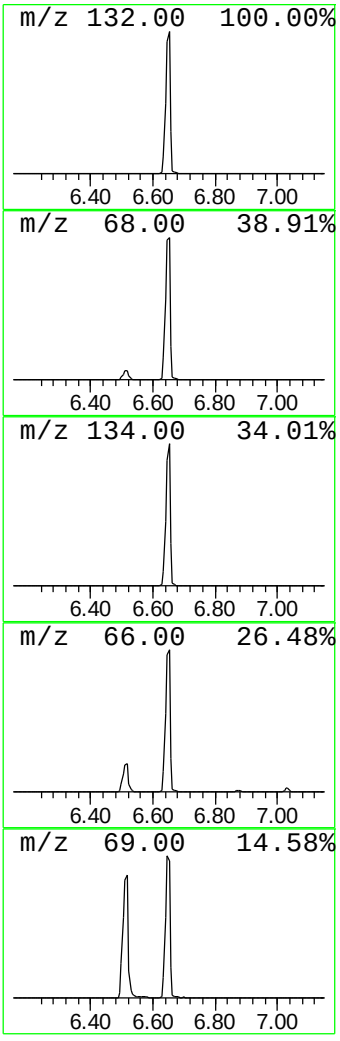
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	80.19 ng	3625860	1,4-Dichlorobenzene-d4	6.87

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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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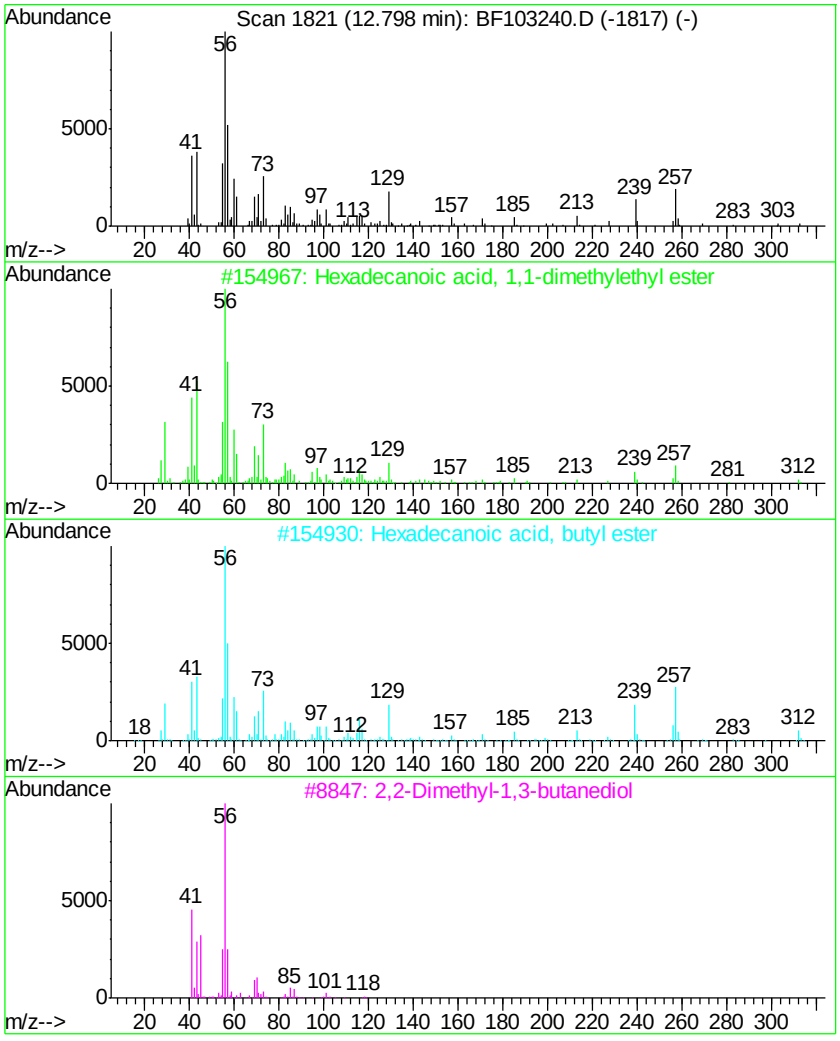
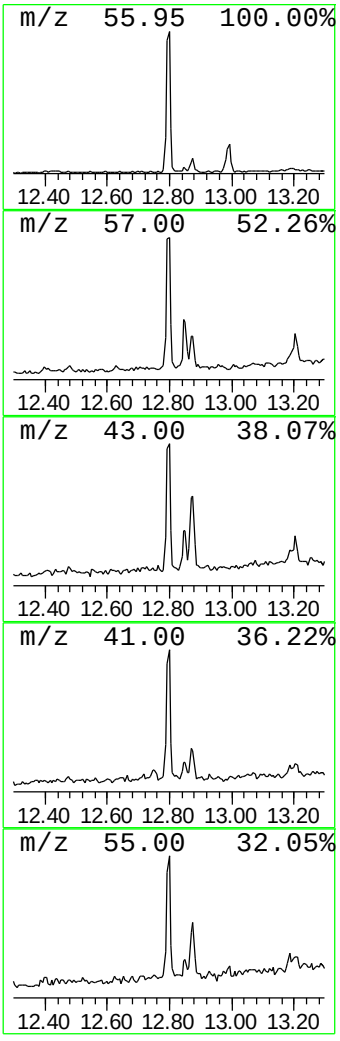
Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	5.89 ng	216401	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	92
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	43
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38
5	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38





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Sample : J1660-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

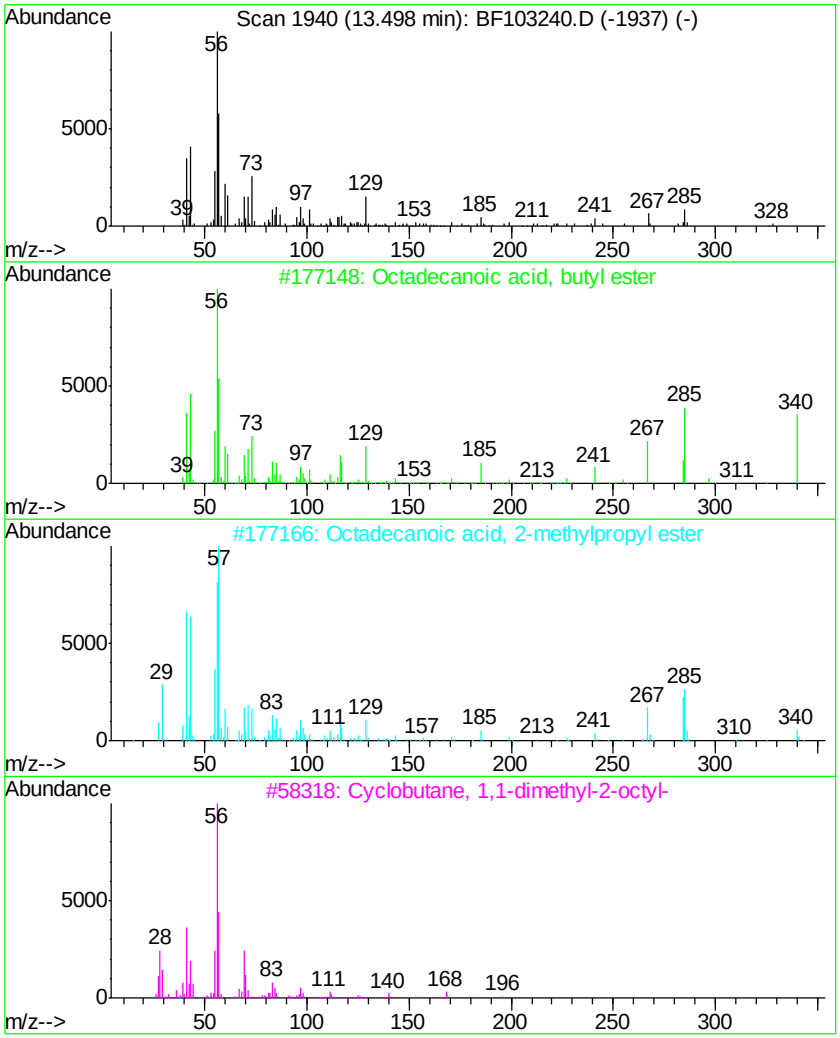
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

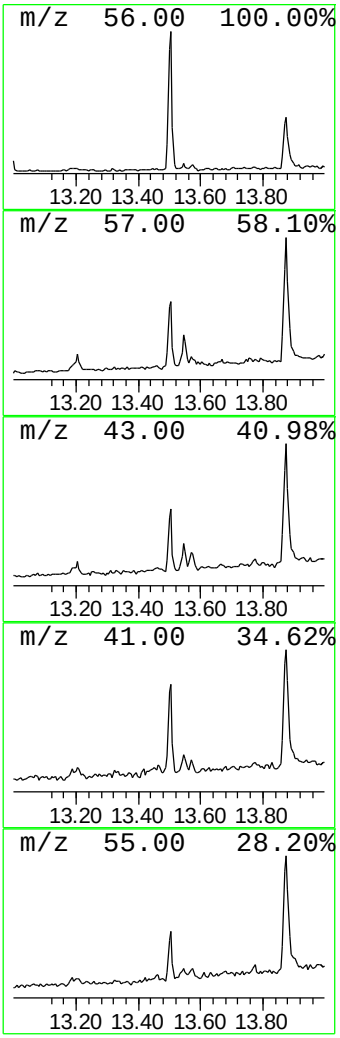
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	4.99 ng	183187	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	55
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	43
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35
5	2-Decene, 9-methyl-, (Z)-	154	C11H22	074630-24-3	32





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Sample : J1660-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-1488

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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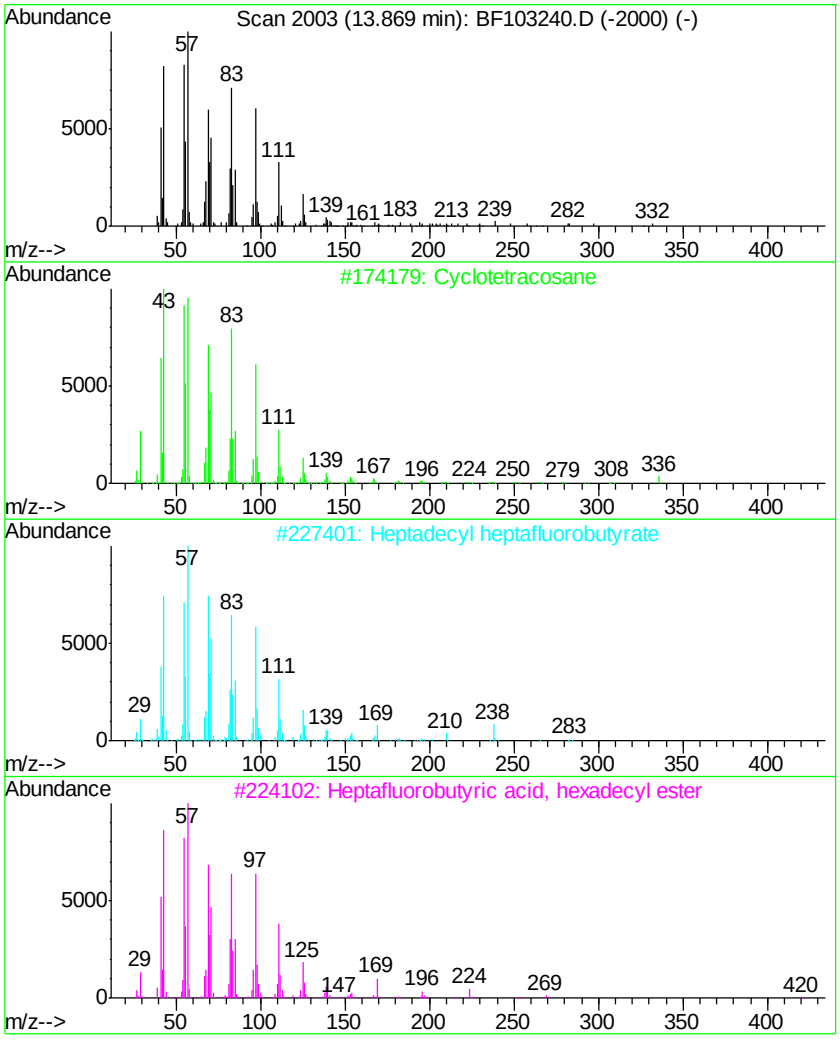
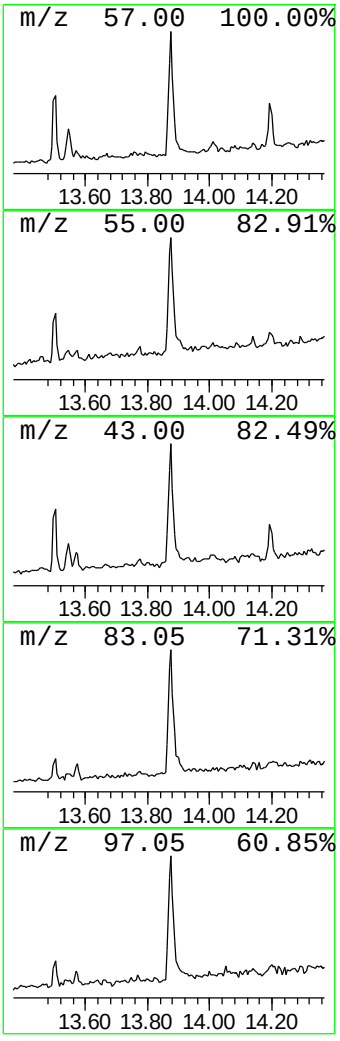
Peak Number 7 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	10.81 ng	396819	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Cyclopentadecane	210	C15H30	000295-48-7	92
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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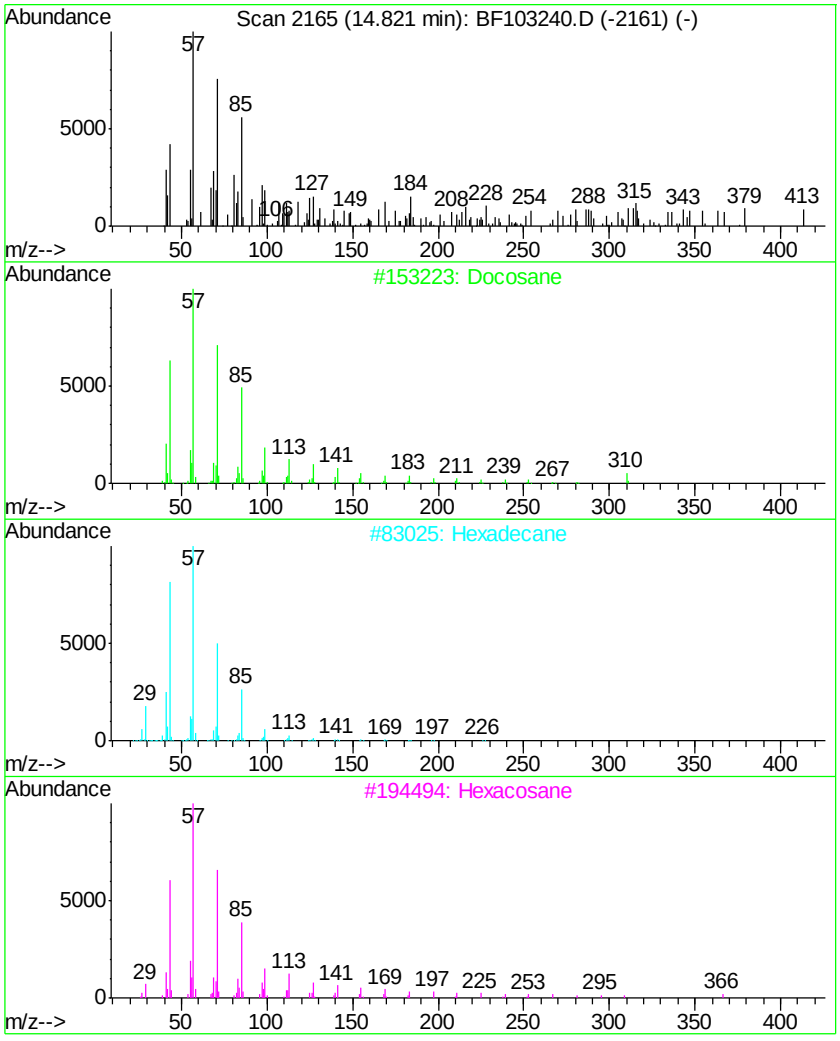
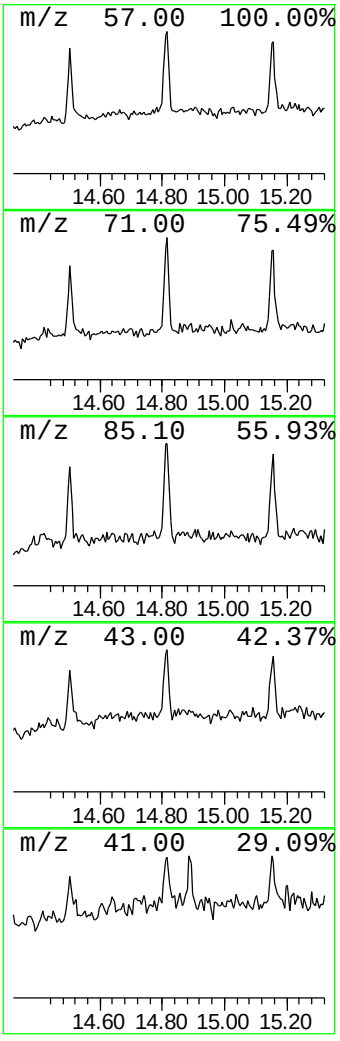
Peak Number 8 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.36 ng	79863	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Hexacosane	366	C26H54	000630-01-3	87
4	Pentacosane	352	C25H52	000629-99-2	83
5	Heneicosane	296	C21H44	000629-94-7	83





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
Butane, 2-methoxy...	2.16	31.4	ng	1422120	1	6.87	904263	20.0
2-Pentanone, 4-hy...	5.12	4.5	ng	201685	1	6.87	904263	20.0
unknown6.65	6.65	80.2	ng	3625860	1	6.87	904263	20.0
Hexadecanoic acid...	12.80	5.9	ng	216401	5	14.06	734408	20.0
Octadecanoic acid...	13.50	5.0	ng	183187	5	14.06	734408	20.0
Cyclotetracosane	13.87	10.8	ng	396819	5	14.06	734408	20.0
Docosane	14.82	2.4	ng	79863	6	15.56	675711	20.0