LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108919.D
Acq On : 11 Sep 2018 3:31
Operator : JU/SJ
Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

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-BF090518.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	4.925	436	440	449	rVB	114362	132059	3.00%	0.480%
2	5.342	507	511	515	rBV	1446795	1371985	31.15%	4.991%
3	6.366	681	685	692	rBV	1209082	995693	22.61%	3.622%
4	6.507	705	709	712	rVB	2879446	2467747	56.04%	8.978%
5	6.736	745	748	752	rBV	1134229	938990	21.32%	3.416%
6	6.895	771	775	779	rBV	3670155	3377789	76.70%	12.289%
7	7.301	838	844	847	rBV	2857482	2685044	60.97%	9.769%
8	8.019	962	966	969	rBV	1362087	1080228	24.53%	3.930%
9	9.095	1145	1149	1152	rBV	4771754	4403839	100.00%	16.022%
10	9.483	1212	1215	1219	rBV	321084	266584	6.05%	0.970%
11	9.771	1260	1264	1267	rBV	1106450	1026654	23.31%	3.735%
12	10.448	1376	1379	1382	rVB	114243	86063	1.95%	0.313%
13	10.554	1393	1397	1403	rBV	1537102	1441047	32.72%	5.243%
14	11.242	1511	1514	1518	rBV	1009388	886377	20.13%	3.225%
15	11.783	1603	1606	1610	rBV	72979	69145	1.57%	0.252%
16	12.348	1699	1702	1711	rBV2	56754	107264	2.44%	0.390%
17	12.830	1779	1784	1787	rBV	3988894	3579065	81.27%	13.021%
18	13.171	1840	1842	1846	rVB	68542	58782	1.33%	0.214%
19	13.742	1935	1939	1946	rBV2	65314	83698	1.90%	0.305%
20	13.871	1957	1961	1965	rVB	1209875	1035927	23.52%	3.769%
21	14.654	2091	2094	2098	rBV	61525	66138	1.50%	0.241%
22	14.724	2103	2106	2110	rVV	256275	247542	5.62%	0.901%
23	14.977	2145	2149	2154	rBV	85599	92458	2.10%	0.336%
24	15.277	2196	2200	2205	rBV	607476	705841	16.03%	2.568%
25	15.336	2206	2210	2216	rVB	89458	117798	2.67%	0.429%
26	15.742	2275	2279	2285	rBV	75100	101494	2.30%	0.369%
27	16.212	2355	2359	2364	rVB	40145	61405	1.39%	0.223%

Sum of corrected areas: 27486656

LSC Report - Integrated Chromatogram

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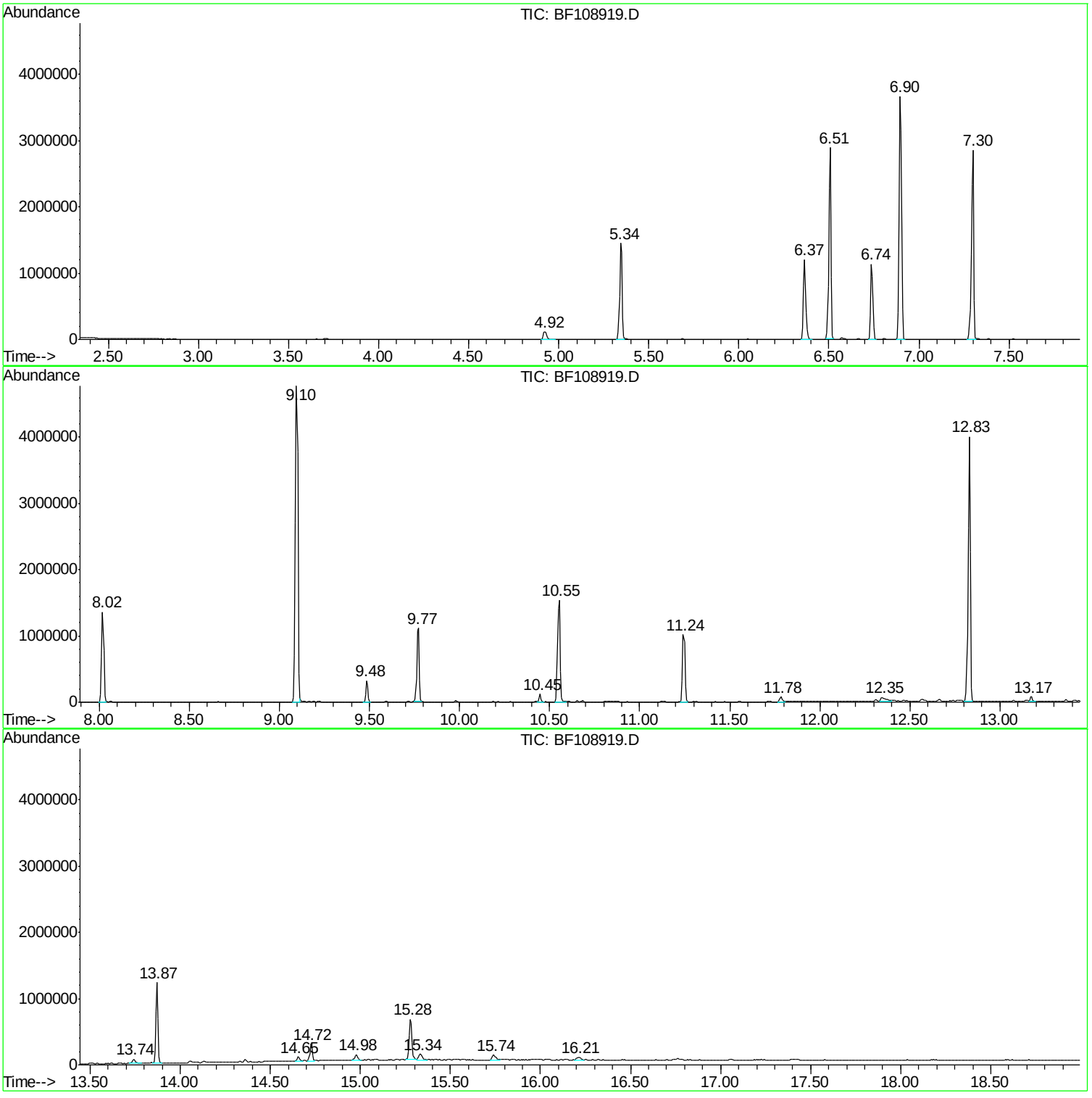
Operator : JU/SJ
Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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\BF091018\
Data File : BF108919.D
Acq On : 11 Sep 2018 3:31
Operator : JU/SJ
Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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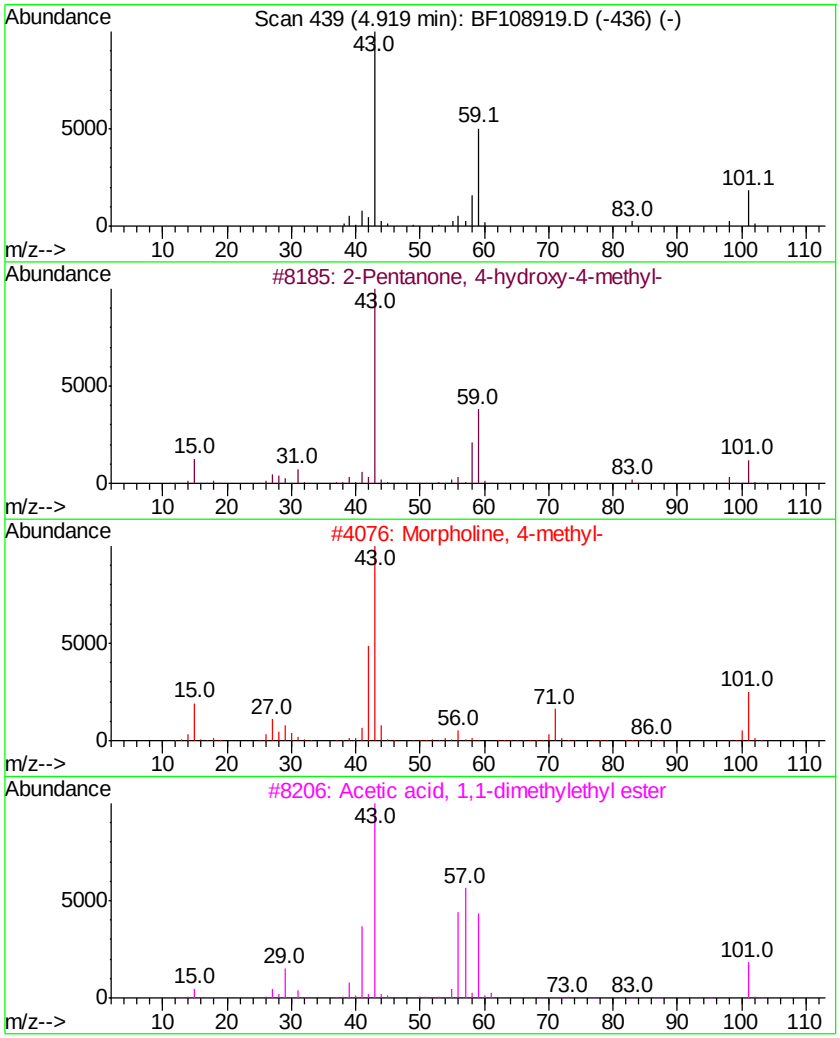
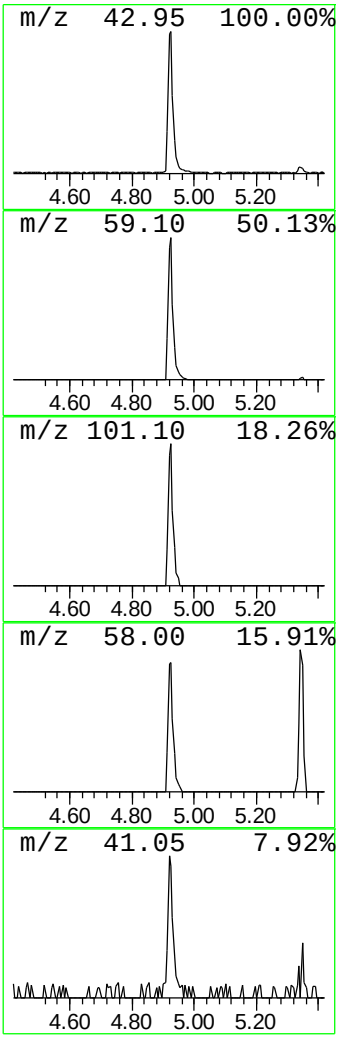
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.81 ng	132059	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9





Library Search Compound Report

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Data File : BF108919.D
Acq On : 11 Sep 2018 3:31
Operator : JU/SJ
Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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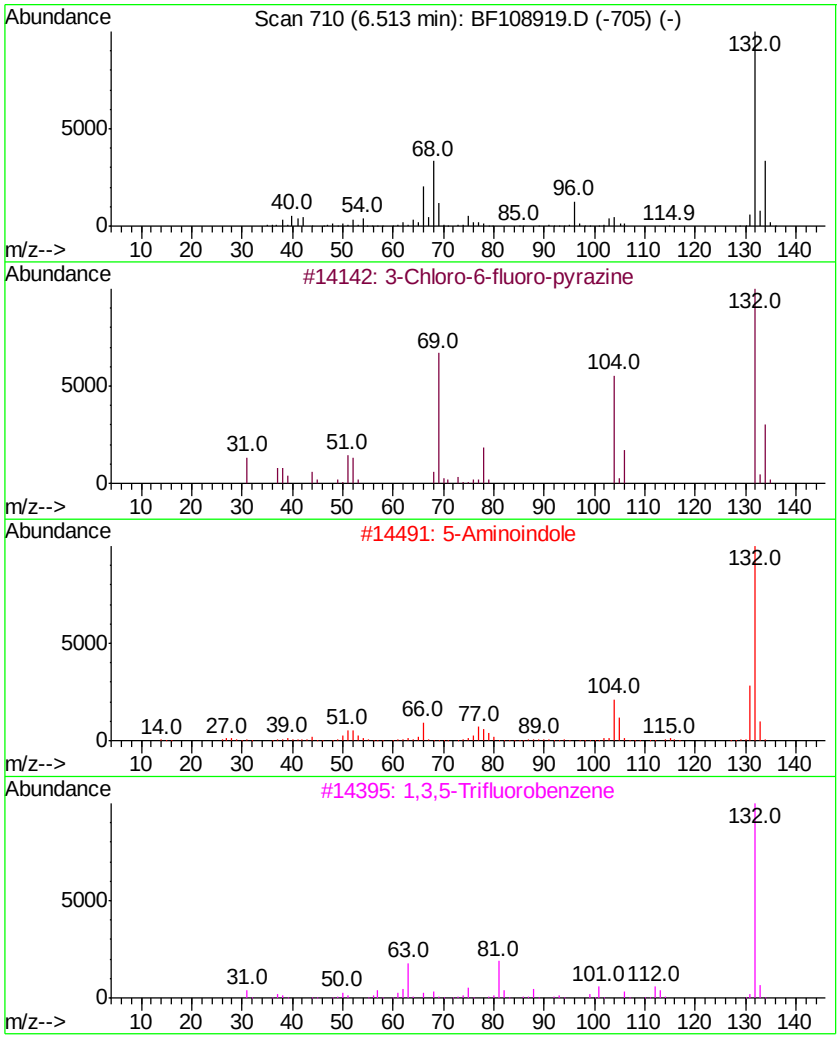
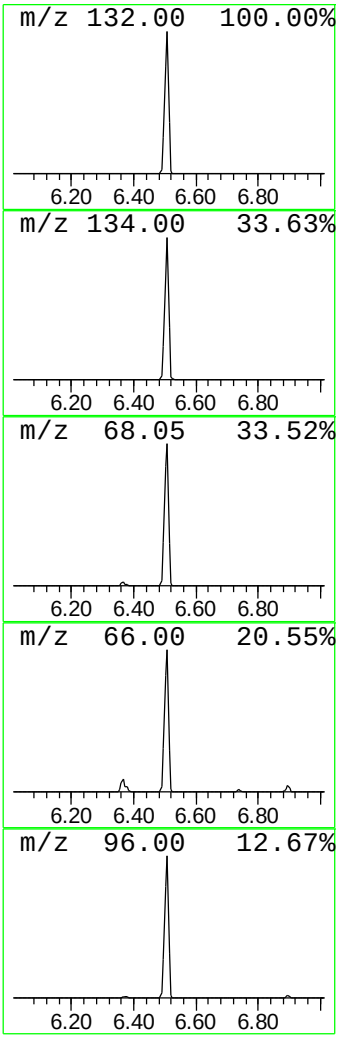
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	52.56 ng	2467750	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108919.D
Acq On : 11 Sep 2018 3:31
Operator : JU/SJ
Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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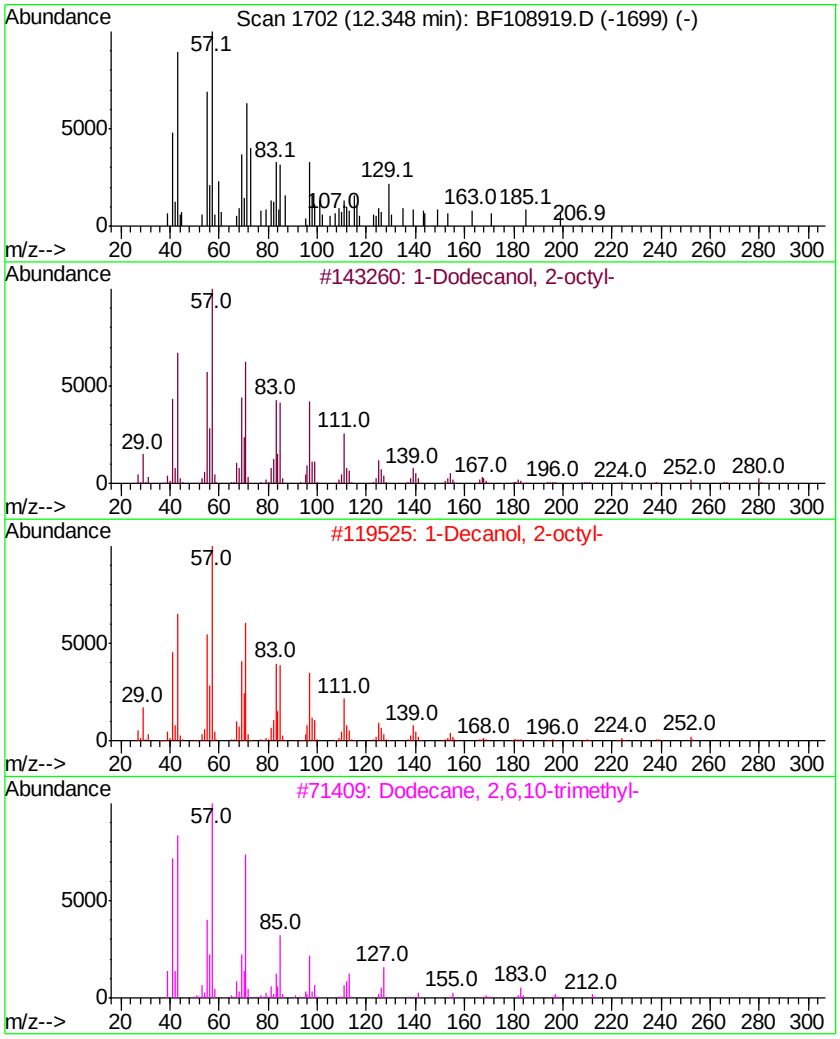
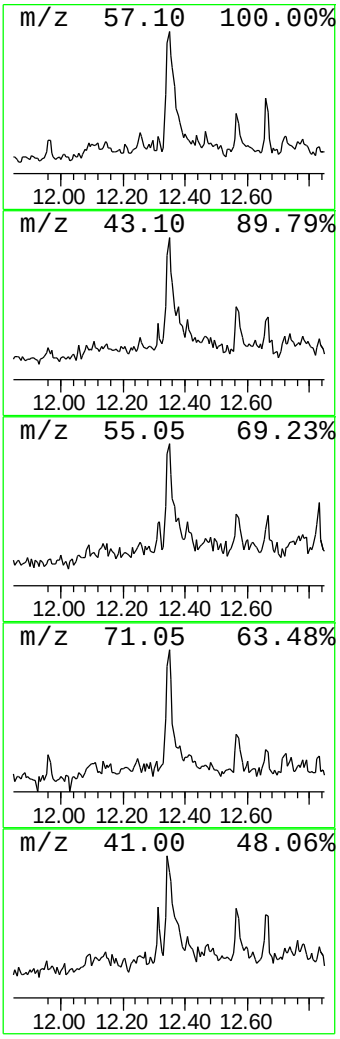
Peak Number 4 unknown12.35 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	2.42 ng	107264	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	43
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	43
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	38
4	Dodecane	170	C12H26	000112-40-3	30
5	Heptacosane	380	C27H56	000593-49-7	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108919.D
Acq On : 11 Sep 2018 3:31
Operator : JU/SJ
Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

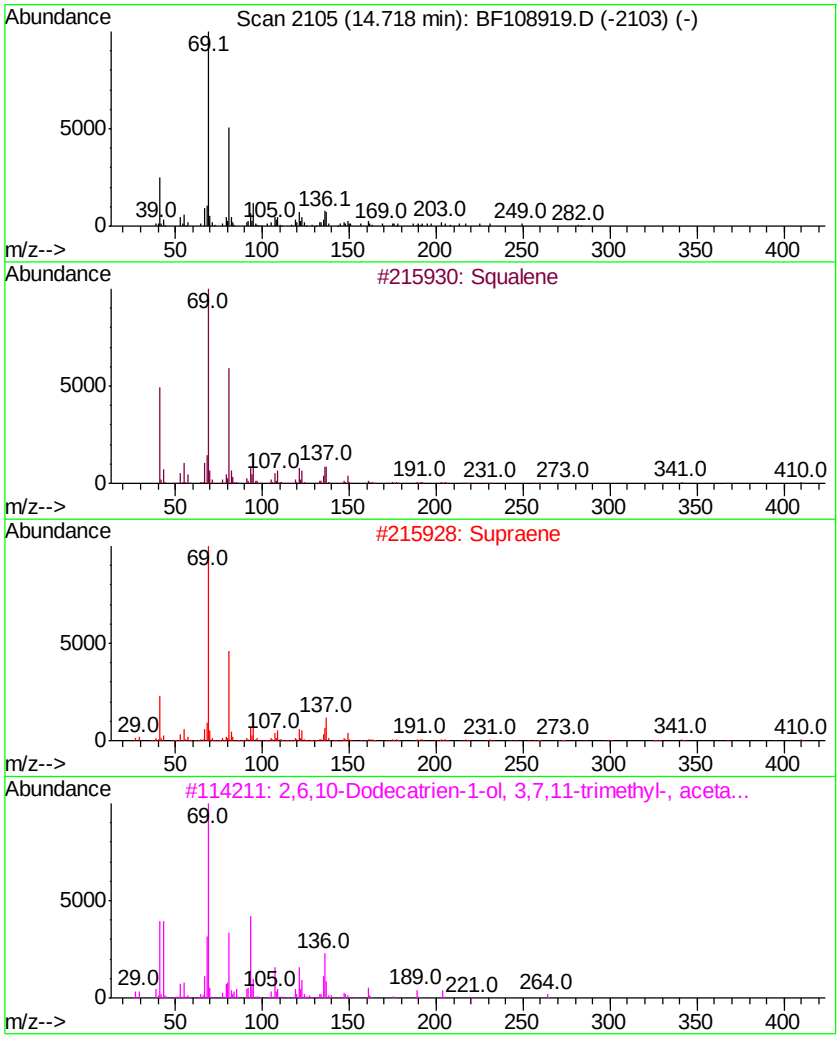
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

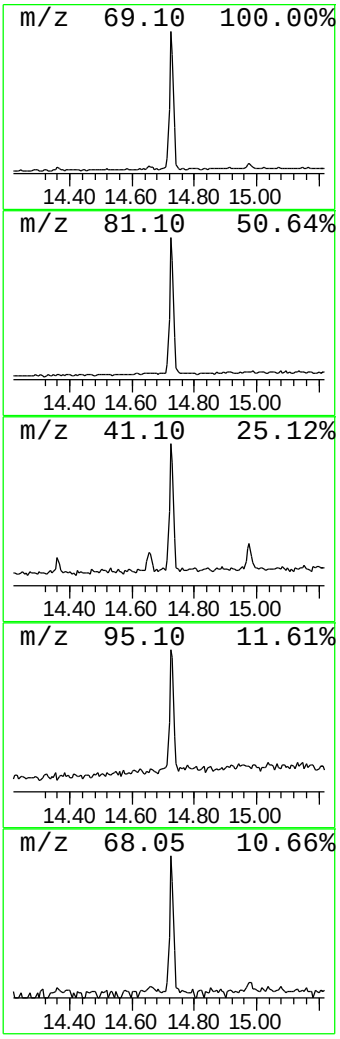
****

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	7.01 ng	247542	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
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Sample : J4830-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

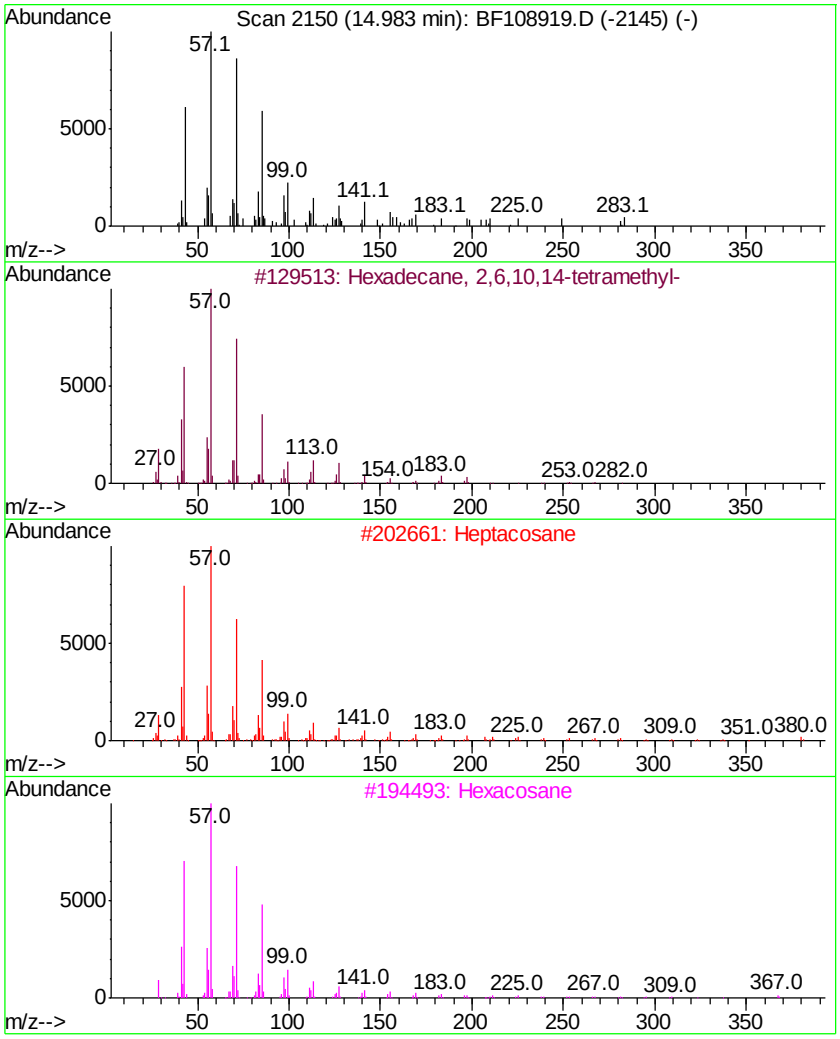
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

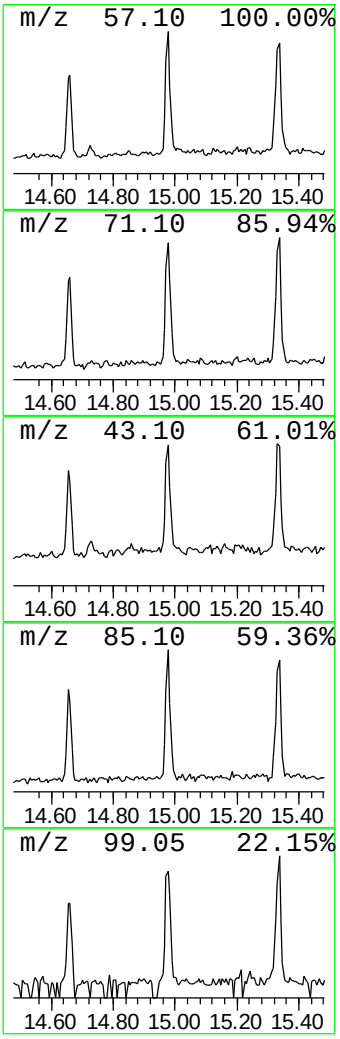
****

Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.62 ng	92458	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	92
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

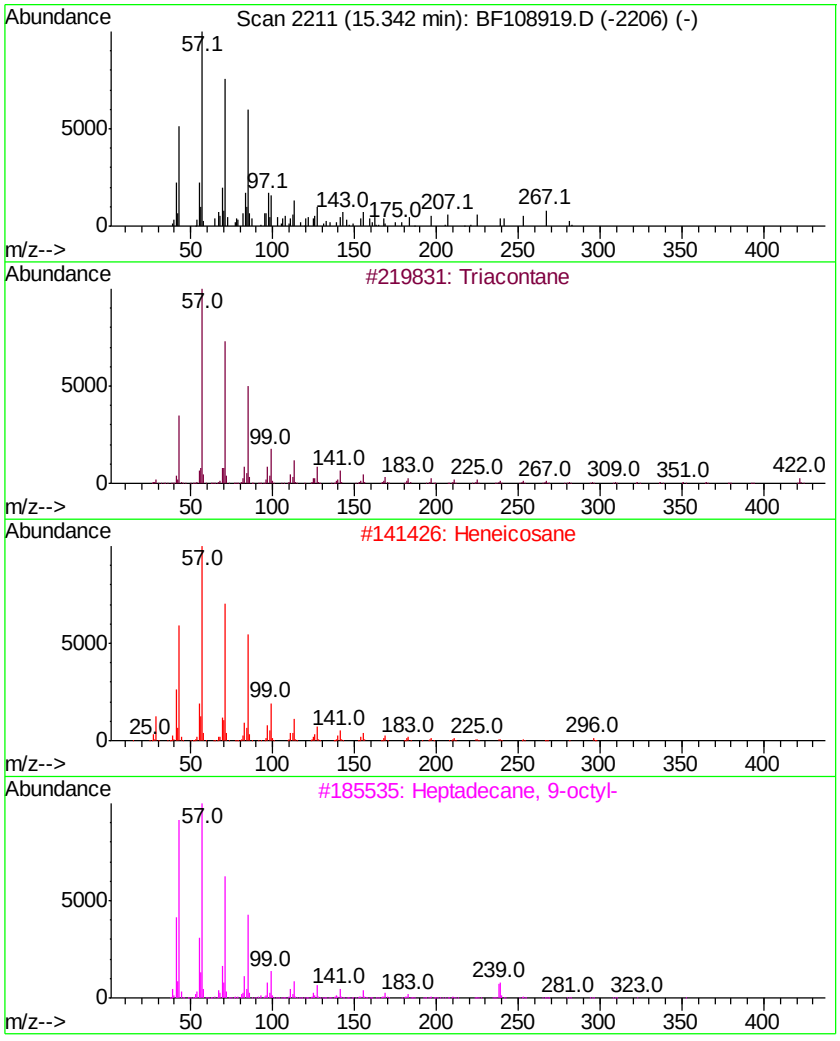
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

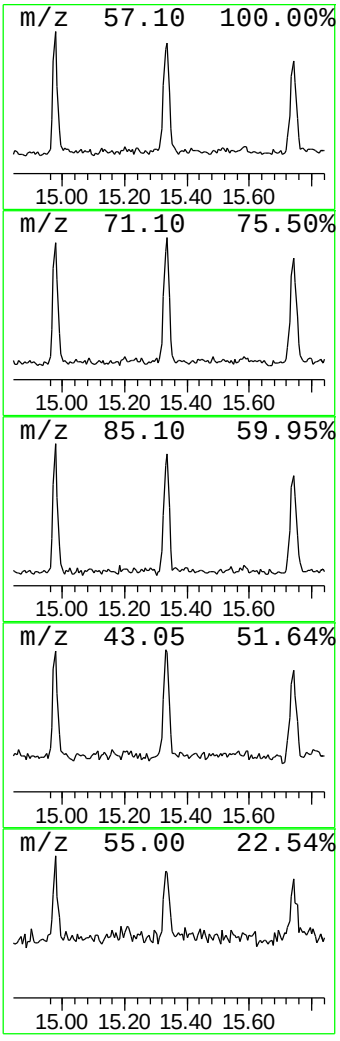
****

Peak Number 7 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	3.34 ng	117798	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	91





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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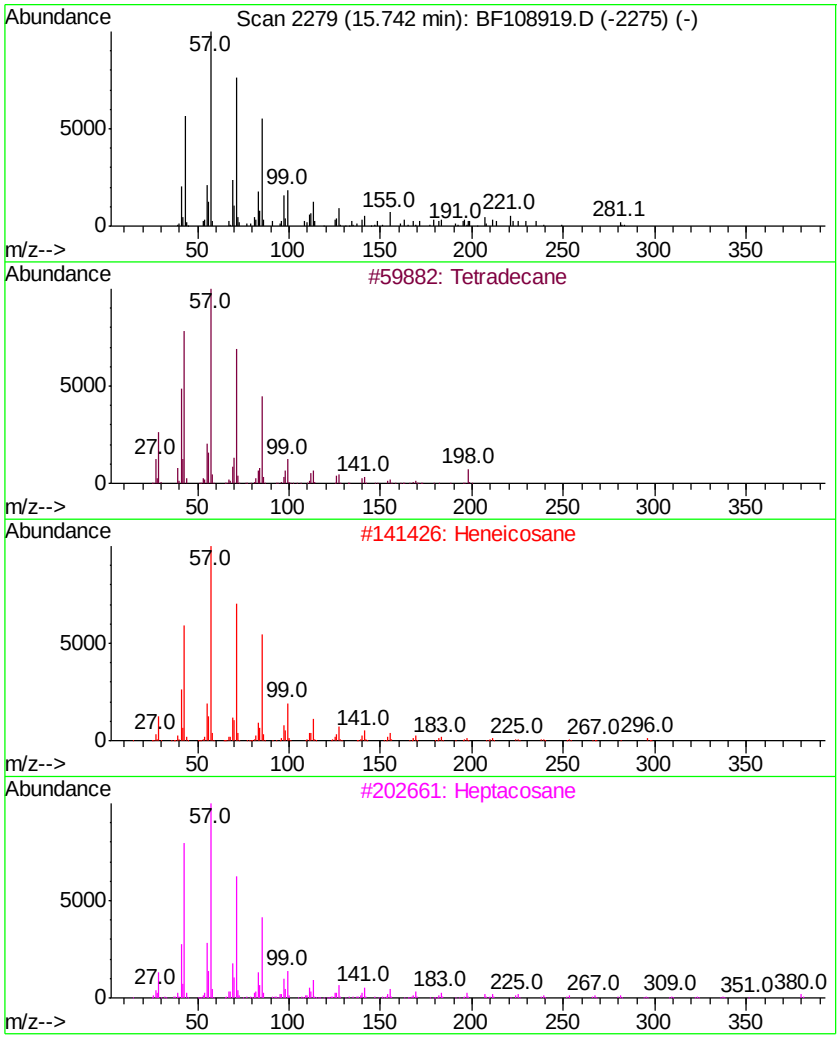
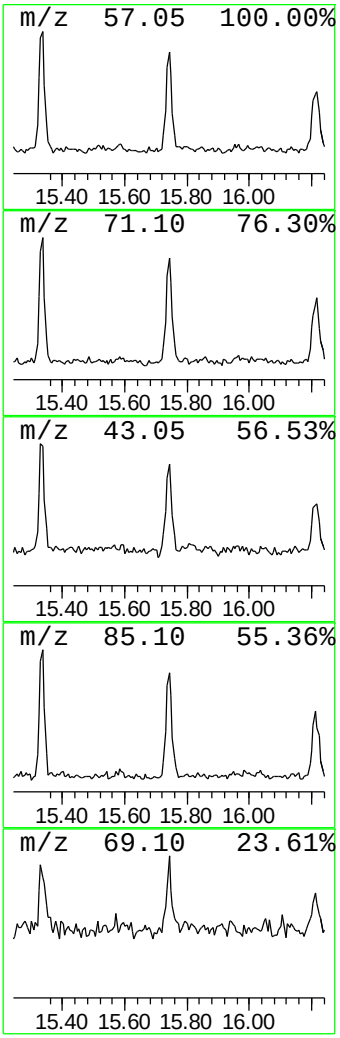
Peak Number 8 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.88 ng	101494	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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
2-Pentanone, 4-hy...	4.92	2.8	ng	132059	1	6.74	938990	20.0
unknown6.51	6.51	52.6	ng	2467750	1	6.74	938990	20.0
unknown12.35	12.35	2.4	ng	107264	4	11.24	886377	20.0
Squalene	14.72	7.0	ng	247542	6	15.28	705841	20.0
Hexadecane, 2,6,1...	14.98	2.6	ng	92458	6	15.28	705841	20.0
Triacontane	15.34	3.3	ng	117798	6	15.28	705841	20.0
Tetradecane	15.74	2.9	ng	101494	6	15.28	705841	20.0