LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097049.D
Acq On : 26 Jul 2017 00:34
Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

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-BF072517.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	2.646	126	129	149	rBV	55335	150468	5.38%	0.663%
2	4.640	465	468	480	rVB	183152	292951	10.47%	1.291%
3	5.098	541	546	560	rBV	2552571	2721014	97.25%	11.992%
4	6.163	722	727	741	rBV	2347824	2797826	100.00%	12.330%
5	6.275	741	746	749	rBV	2610507	2585247	92.40%	11.393%
6	6.498	780	784	790	rBV	907490	761412	27.21%	3.356%
7	6.657	806	811	814	rBV	2070645	1982886	70.87%	8.739%
8	6.922	851	856	861	rBV	147167	125001	4.47%	0.551%
9	7.069	876	881	884	rBV	1721167	1606081	57.40%	7.078%
10	7.198	901	903	913	rVB	24015	28282	1.01%	0.125%
11	7.781	998	1002	1006	rBV	1194814	959901	34.31%	4.230%
12	8.063	1045	1050	1055	rBV	31720	33542	1.20%	0.148%
13	8.863	1181	1186	1189	rBV	2594708	2388740	85.38%	10.527%
14	9.257	1250	1253	1256	rVB	340285	239704	8.57%	1.056%
15	9.528	1295	1299	1303	rBV	899868	788293	28.18%	3.474%
16	9.981	1374	1376	1379	rVB	97674	74956	2.68%	0.330%
17	10.198	1408	1413	1418	rBV	33751	53749	1.92%	0.237%
18	10.239	1418	1420	1425	rVB2	22966	28435	1.02%	0.125%
19	10.310	1428	1432	1436	rVV	1232062	1090812	38.99%	4.807%
20	10.451	1453	1456	1463	rBV	135556	159448	5.70%	0.703%
21	10.645	1485	1489	1493	rBV3	20732	33462	1.20%	0.147%
22	10.898	1527	1532	1535	rBV	66784	60757	2.17%	0.268%
23	10.998	1543	1549	1553	rBV	751969	642037	22.95%	2.829%
24	11.322	1601	1604	1609	rVB2	29530	28671	1.02%	0.126%
25	11.557	1641	1644	1651	rBV2	179883	163474	5.84%	0.720%
26	12.251	1759	1762	1767	rBV6	26661	42745	1.53%	0.188%
27	12.333	1774	1776	1782	rBV4	38956	53230	1.90%	0.235%
28	12.427	1789	1792	1795	rBV	39428	35817	1.28%	0.158%
29	12.580	1814	1818	1822	rBV	1527513	1567527	56.03%	6.908%
30	12.757	1846	1848	1853	rBV6	25579	34706	1.24%	0.153%
31	13.498	1971	1974	1980	rVB3	140666	175700	6.28%	0.774%
32	13.621	1991	1995	2002	rBV	563638	563980	20.16%	2.485%
33	14.127	2079	2081	2088	rVB3	95040	124799	4.46%	0.550%
34	14.974	2222	2225	2229	rBV	270365	295428	10.56%	1.302%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097049.D
Acq On : 26 Jul 2017 00:34
Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CEMETERY-6-(0-2)

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

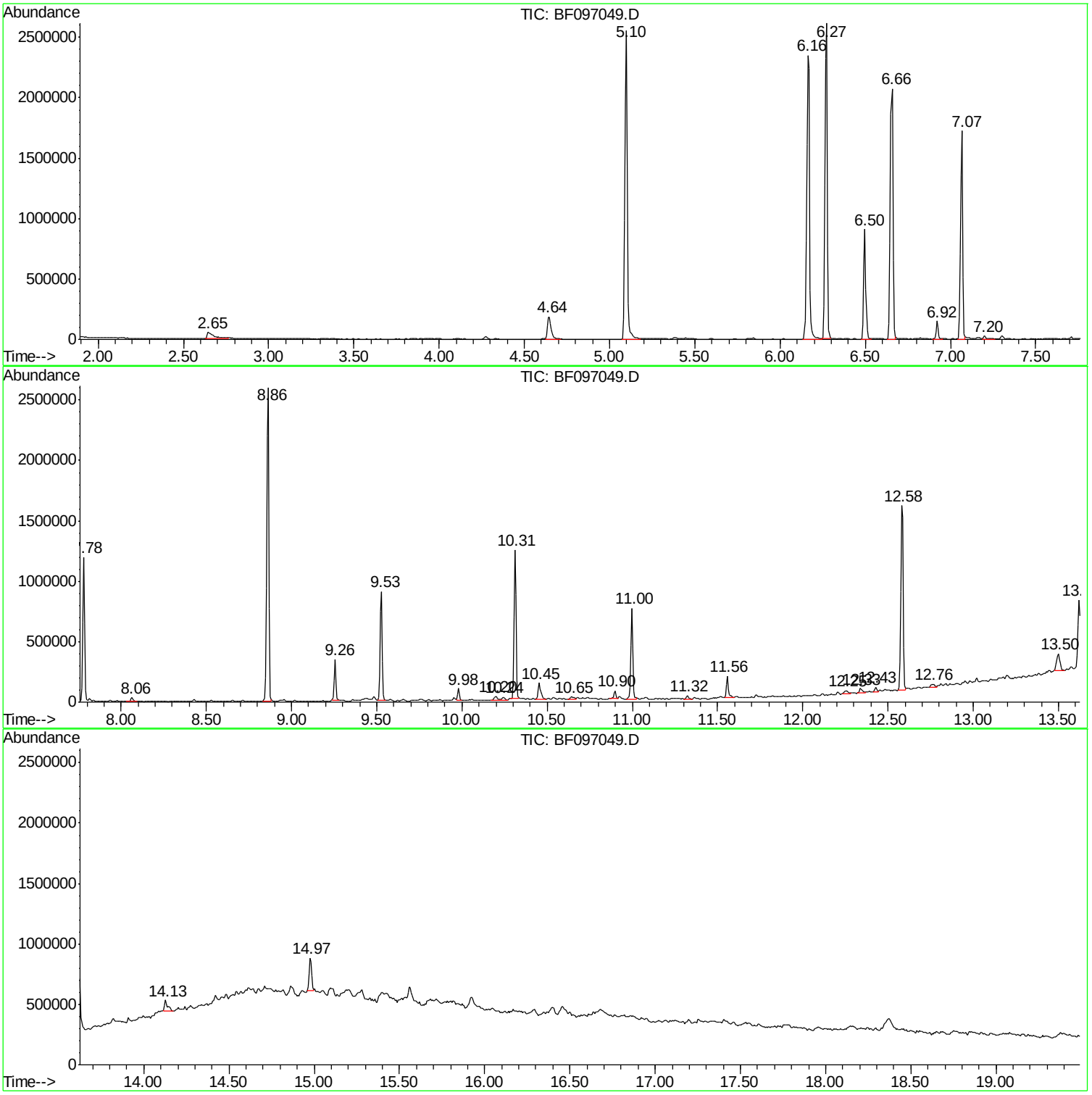
Sum of corrected areas: 22691081

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097049.D
Acq On : 26 Jul 2017 00:34
Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097049.D
Acq On : 26 Jul 2017 00:34
Operator : SJ/JU
Sample : I4359-11
Misc :
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Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

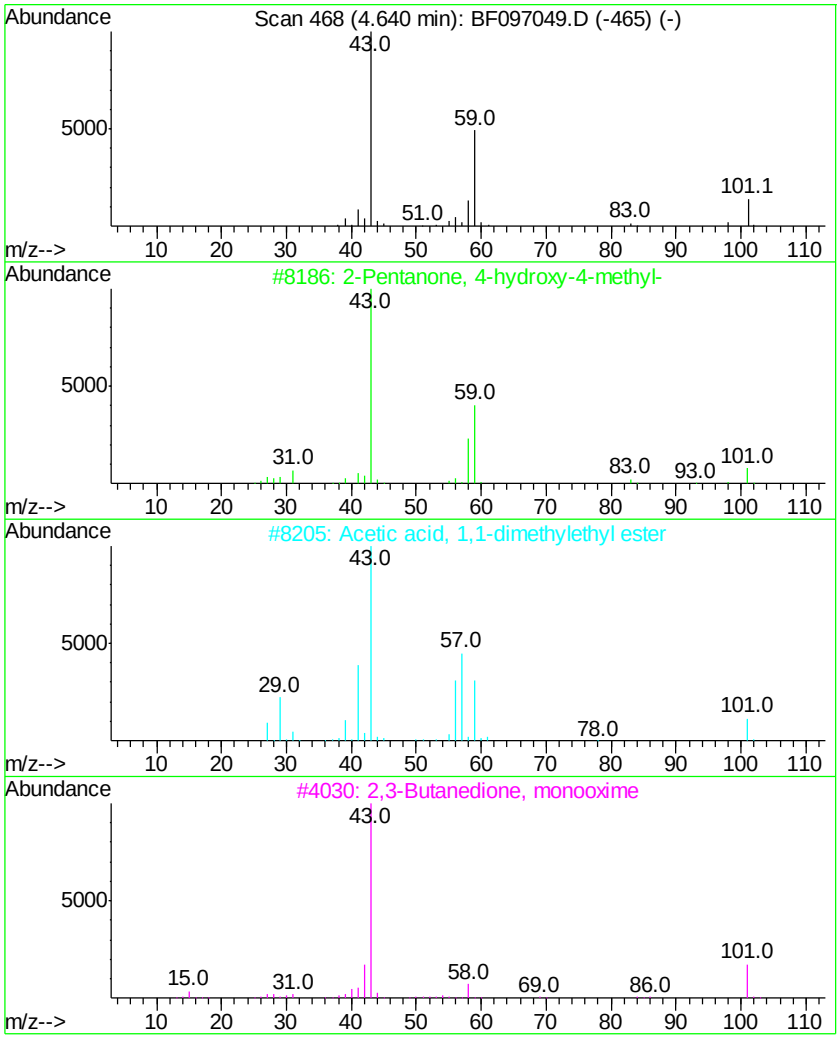
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

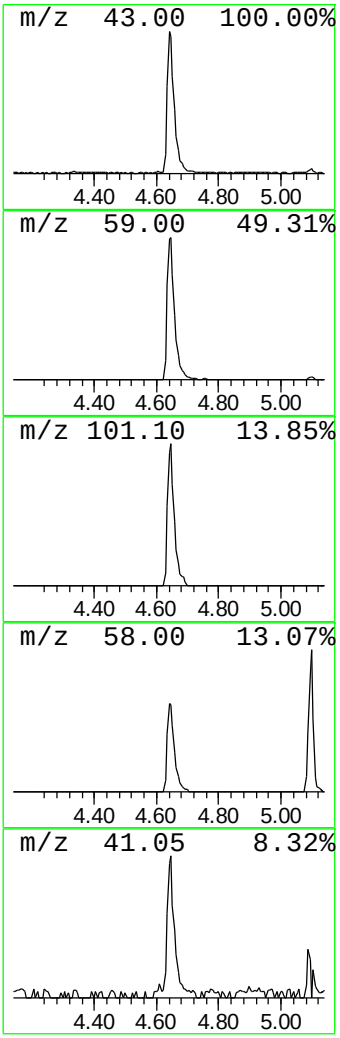
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	7.69 ng	292951	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097049.D
Acq On : 26 Jul 2017 00:34
Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

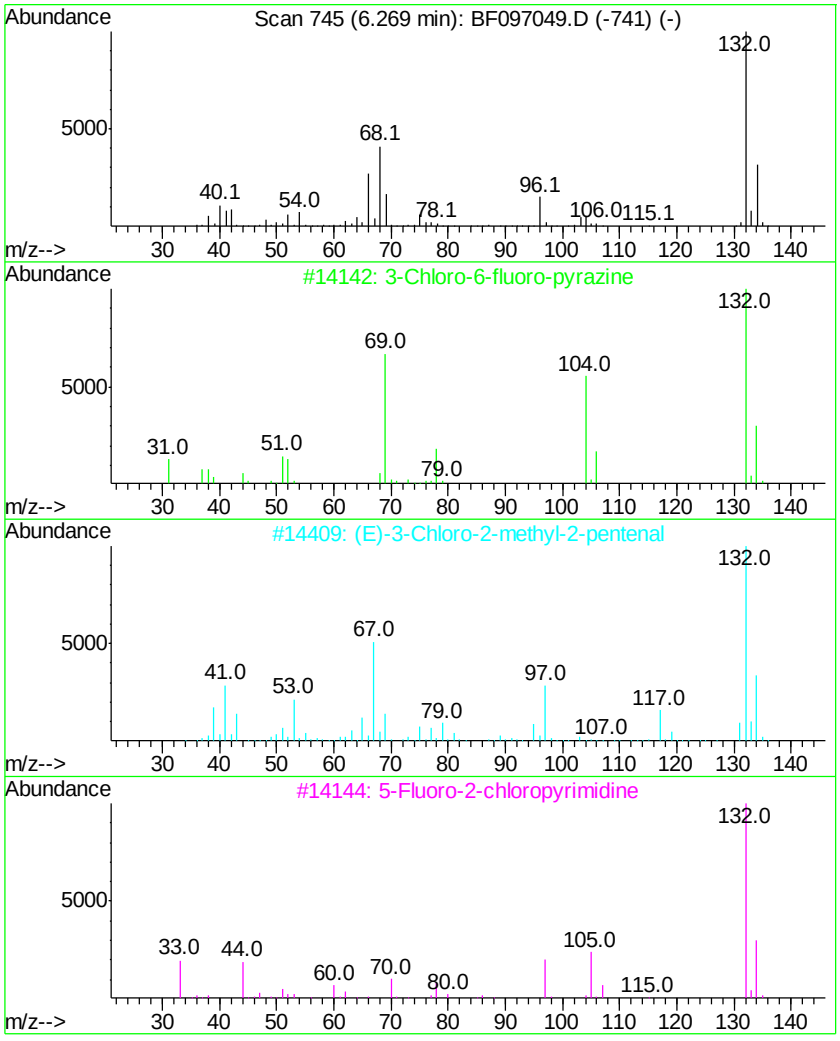
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

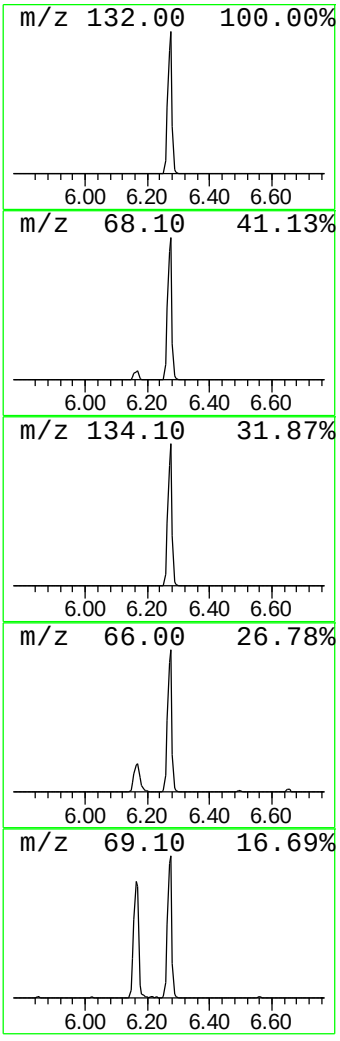
****

Peak Number 3 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	67.91 ng	2585250	1,4-Dichlorobenzene-d4	6.50

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Data File : BF097049.D
Acq On : 26 Jul 2017 00:34
Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

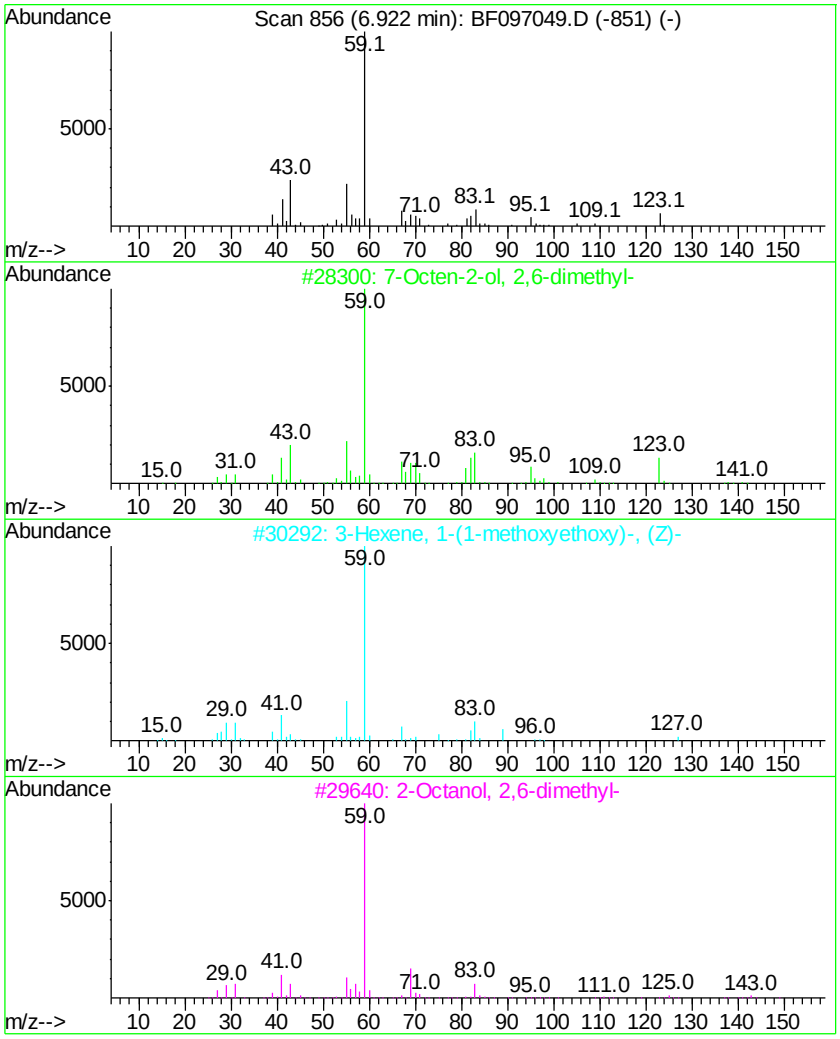
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

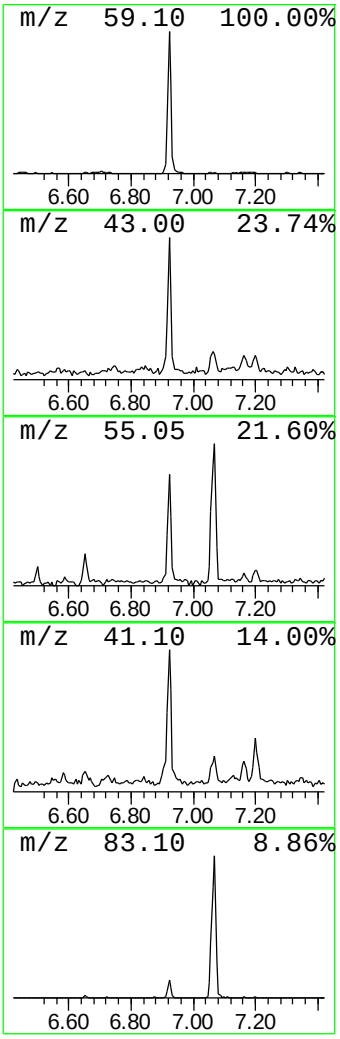
****

Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	3.28 ng	125001	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
2	3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-96-4	56
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097049.D
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Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

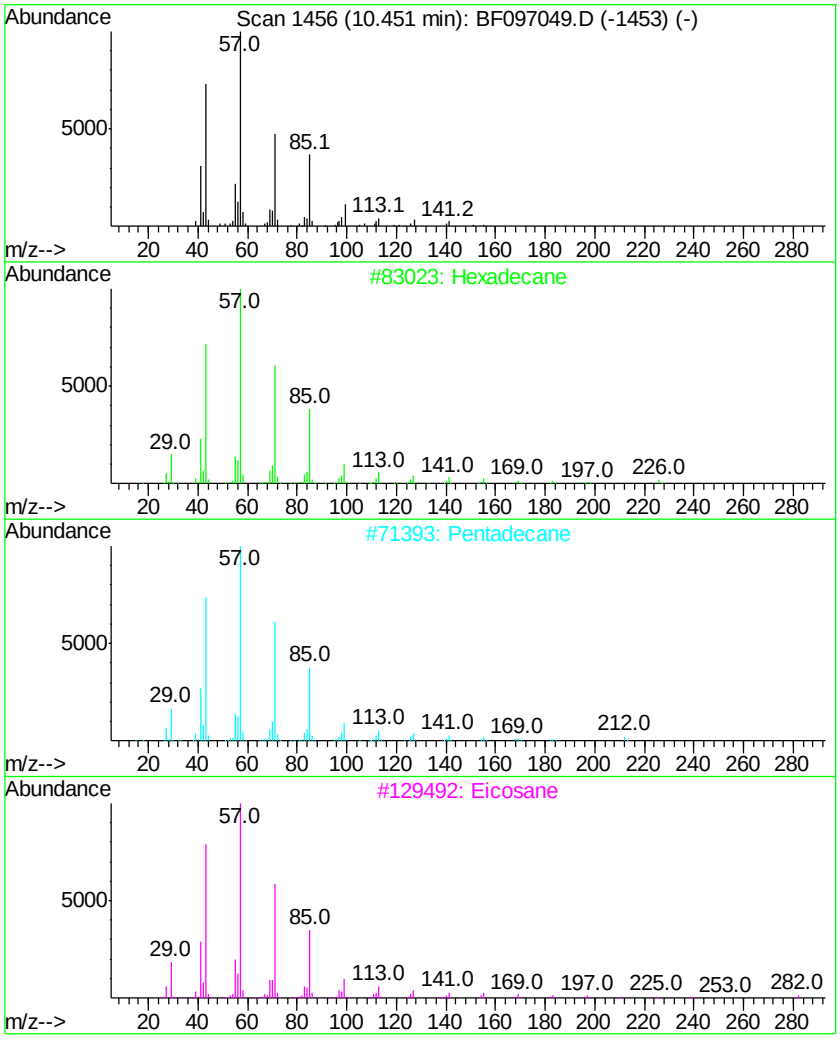
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

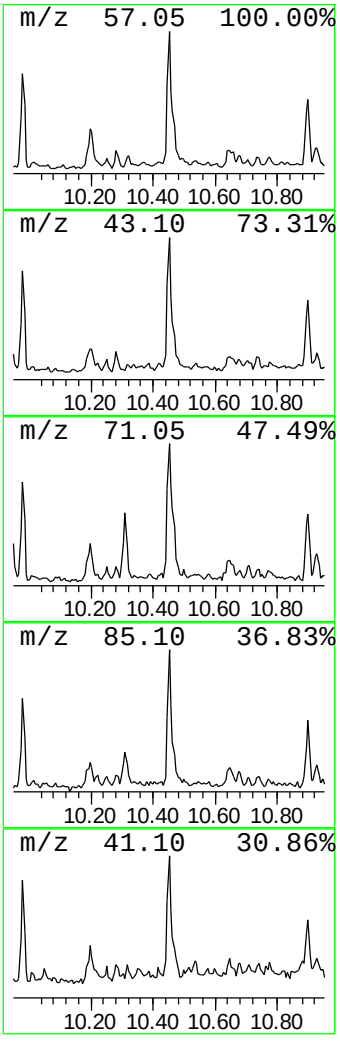
****

Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	4.97 ng	159448	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Eicosane	282	C20H42	000112-95-8	86
4	Heneicosane	296	C21H44	000629-94-7	86
5	Nonadecane	268	C19H40	000629-92-5	86





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

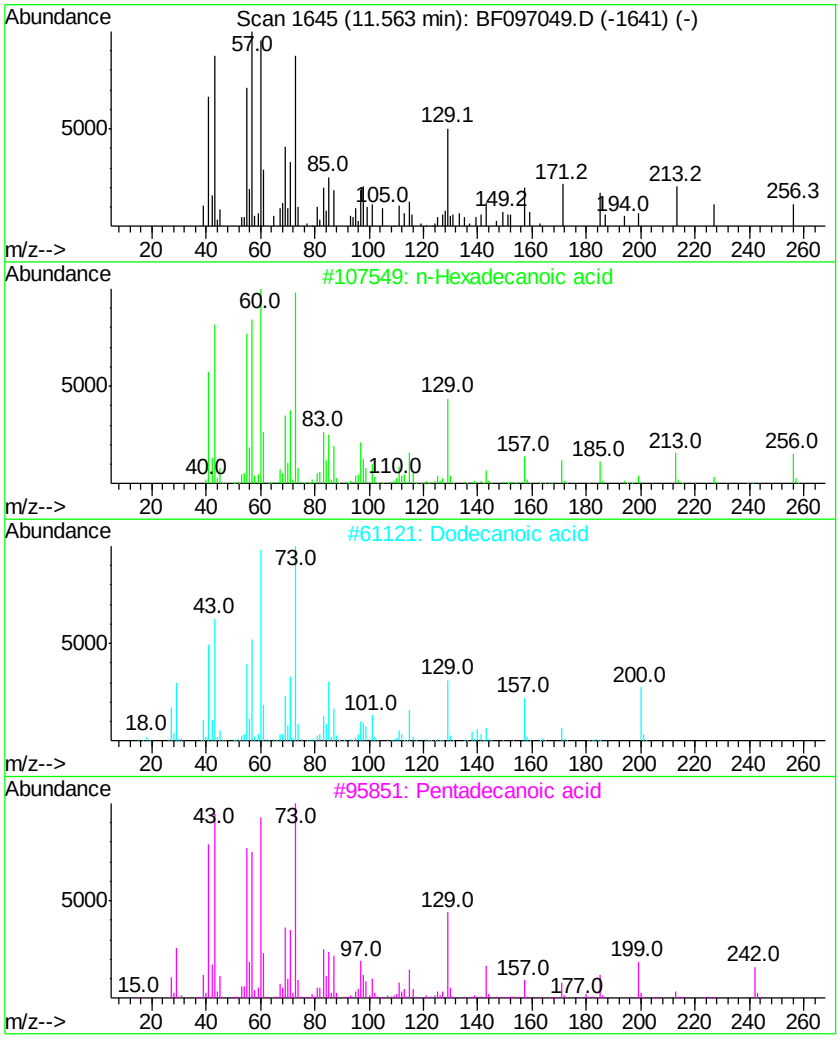
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

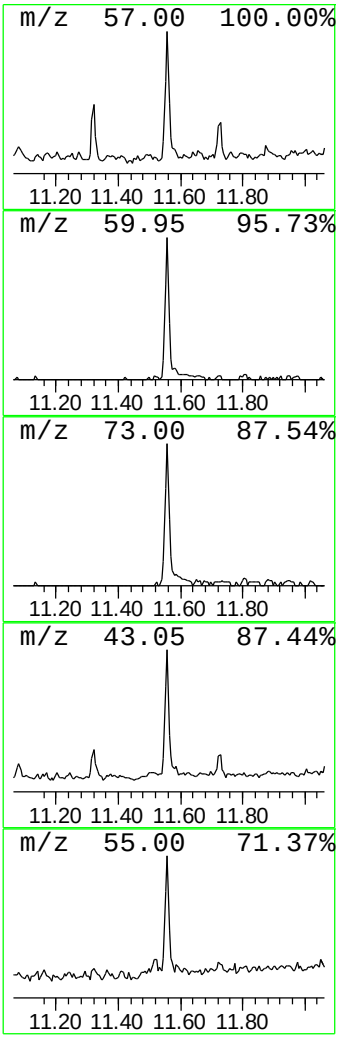
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	5.09 ng	163474	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Dodecanoic acid	200	C12H24O2	000143-07-7	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

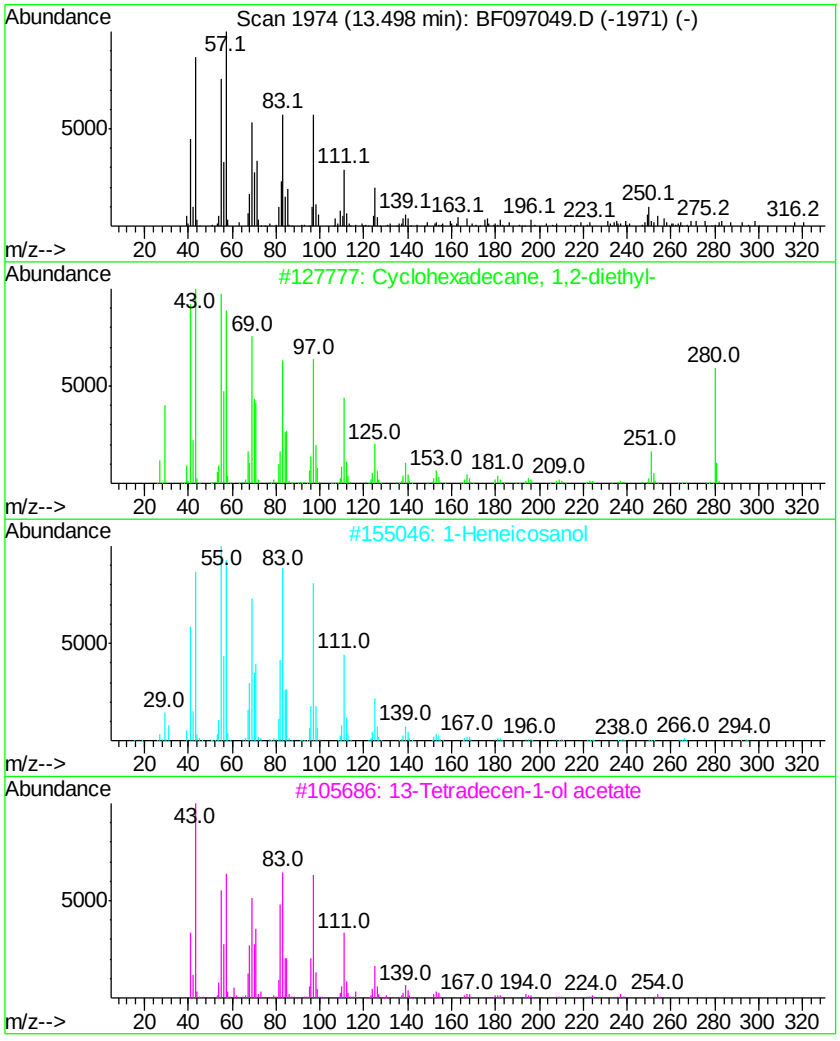
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

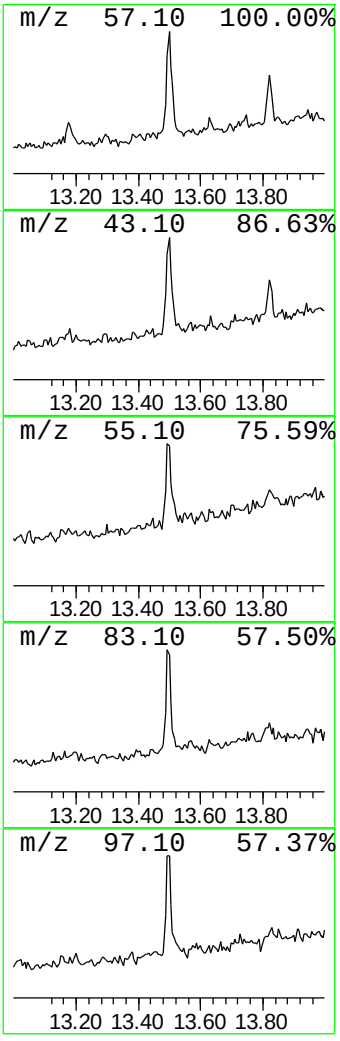
****

Peak Number 8 Cyclohexadecane, 1,2-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	6.23 ng	175700	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
5	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	90





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Operator : SJ/JU
Sample : I4359-11
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-6-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

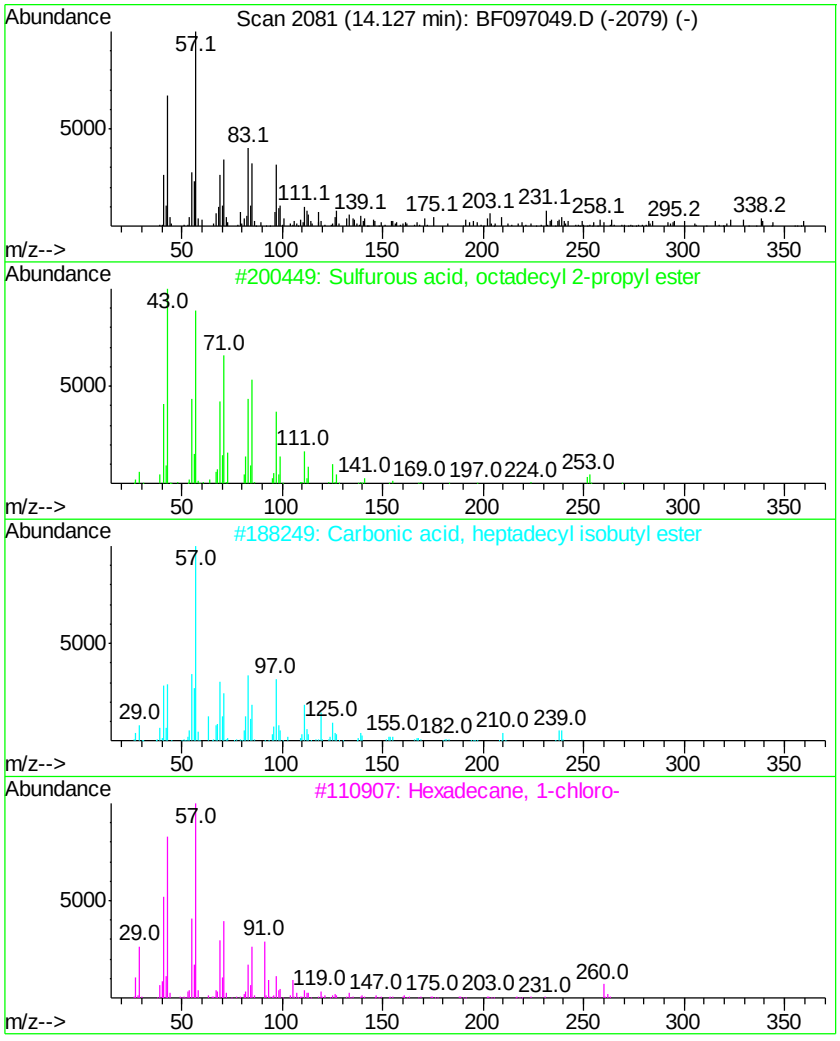
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

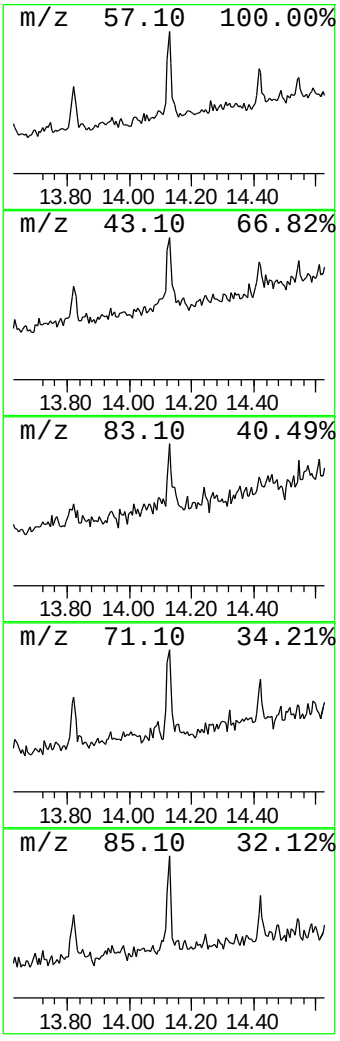
****

Peak Number 9 Sulfurous acid, octadecyl 2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	4.43 ng	124799	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	52
2	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	50
3	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	43
4	Eicosane	282	C20H42	000112-95-8	35
5	1-Tridecene	182	C13H26	002437-56-1	30





Tentatively Identified Compound (LSC) summary

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Operator : SJ/JU
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.64	7.7	ng	292951	1	6.50	761412	20.0
unknown6.27	6.27	67.9	ng	2585250	1	6.50	761412	20.0
7-Octen-2-ol, 2,6...	6.92	3.3	ng	125001	1	6.50	761412	20.0
Hexadecane	10.45	5.0	ng	159448	4	11.00	642037	20.0
n-Hexadecanoic acid	11.56	5.1	ng	163474	4	11.00	642037	20.0
Cyclohexadecane, ...	13.50	6.2	ng	175700	5	13.62	563980	20.0
Sulfurous acid, o...	14.13	4.4	ng	124799	5	13.62	563980	20.0