LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088064.D
Acq On : 16 Jun 2016 5:54
Operator : UM/SJ
Sample : H3570-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-COMP

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-BF060716.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	1.701	8	10	18	rVB	136874	303004	14.09%	1.382%
2	1.815	18	20	31	rVV	1294554	2142006	99.58%	9.772%
3	1.953	31	32	72	rVB3	78479	379854	17.66%	1.733%
4	4.913	289	291	299	rBV	88541	128404	5.97%	0.586%
5	5.336	325	328	330	rBV	1923807	1964229	91.31%	8.961%
6	6.387	417	420	422	rBV	1808830	2145189	99.73%	9.787%
7	6.513	428	431	433	rBV	1851592	2151079	100.00%	9.814%
8	6.742	448	451	453	rBV	720565	600569	27.92%	2.740%
9	6.902	462	465	467	rBV	1479339	1669041	77.59%	7.614%
10	7.313	498	501	503	rBV	1263444	1424952	66.24%	6.501%
11	8.033	561	564	566	rBV	593866	785122	36.50%	3.582%
12	9.108	655	658	660	rBV	2314040	2105462	97.88%	9.605%
13	9.508	690	693	695	rBV	411905	424700	19.74%	1.938%
14	9.782	714	717	719	rVB	893122	834219	38.78%	3.806%
15	9.885	723	726	728	rBB	22818	32461	1.51%	0.148%
16	10.216	754	755	757	rVB	41571	40913	1.90%	0.187%
17	10.433	772	774	778	rBV	15261	28793	1.34%	0.131%
18	10.571	783	786	788	rBV	913582	1119819	52.06%	5.109%
19	10.696	795	797	801	rBV	40542	66959	3.11%	0.305%
20	11.142	834	836	837	rBV	24141	26702	1.24%	0.122%
21	11.256	844	846	849	rVB	794012	682168	31.71%	3.112%
22	11.496	865	867	871	rBV	44676	64627	3.00%	0.295%
23	12.319	937	939	945	rBV	75682	127082	5.91%	0.580%
24	12.845	982	985	987	rBV	1542555	1392330	64.73%	6.352%
25	13.199	1014	1016	1019	rBV	33810	46770	2.17%	0.213%
26	13.748	1062	1064	1074	rBV	33030	82773	3.85%	0.378%
27	13.885	1074	1076	1079	rVV	496329	573345	26.65%	2.616%
28	15.291	1196	1199	1202	rBV	453555	576856	26.82%	2.632%

Sum of corrected areas: 21919428

LSC Report - Integrated Chromatogram

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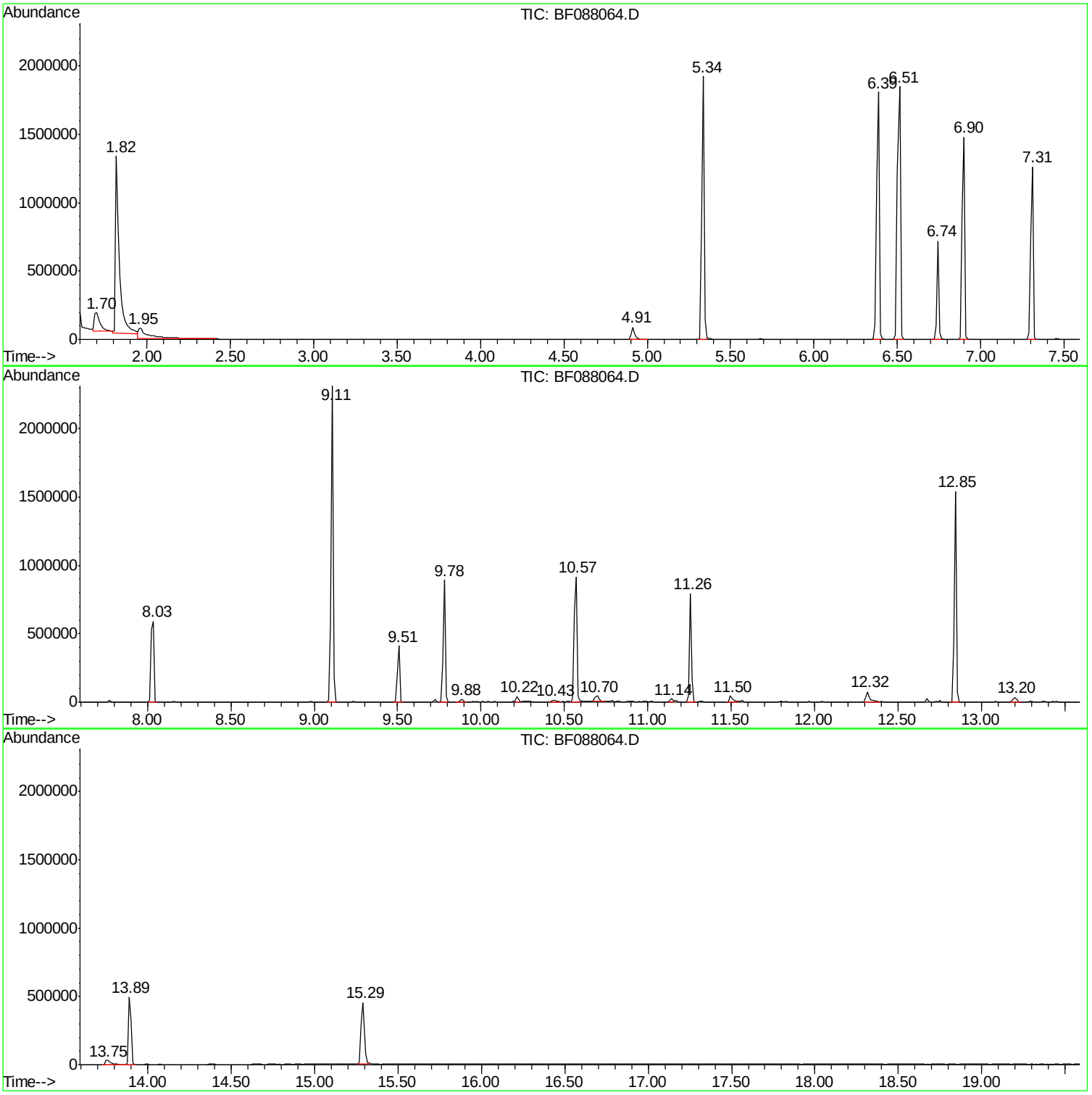
Operator : UM/SJ
Sample : H3570-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061516\
Data File : BF088064.D
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ClientSampleId : SB-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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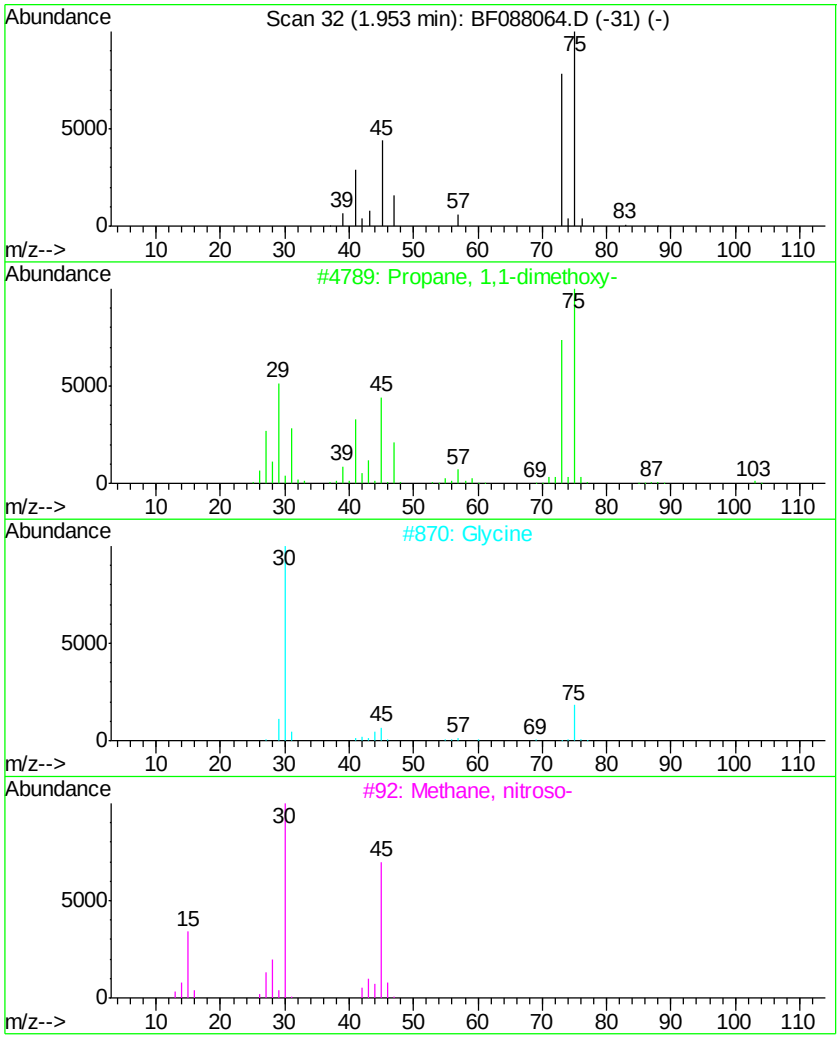
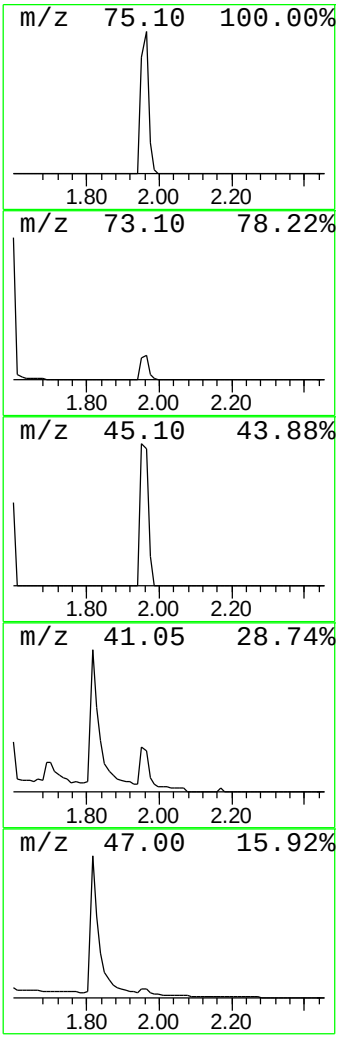
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.95	12.65 ng	379854	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	Glycine	75	C2H5NO2	000056-40-6	7
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	4
5	Ethanethioamide	75	C2H5NS	000062-55-5	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088064.D
Acq On : 16 Jun 2016 5:54
Operator : UM/SJ
Sample : H3570-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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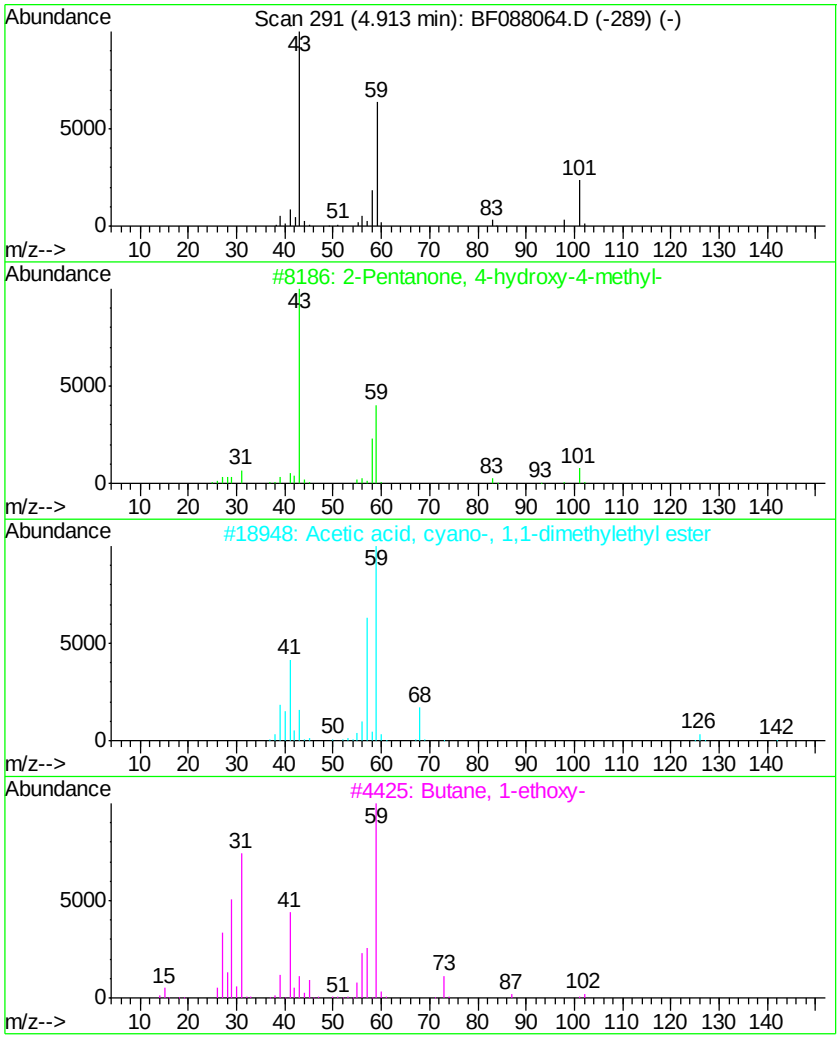
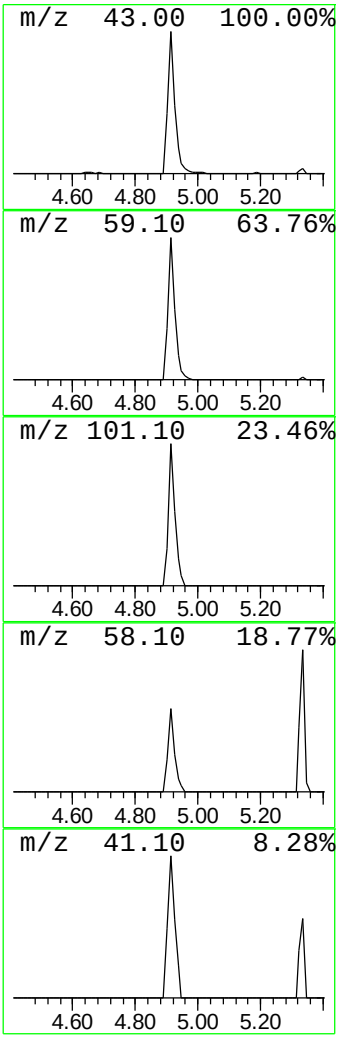
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.28 ng	128404	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088064.D
Acq On : 16 Jun 2016 5:54
Operator : UM/SJ
Sample : H3570-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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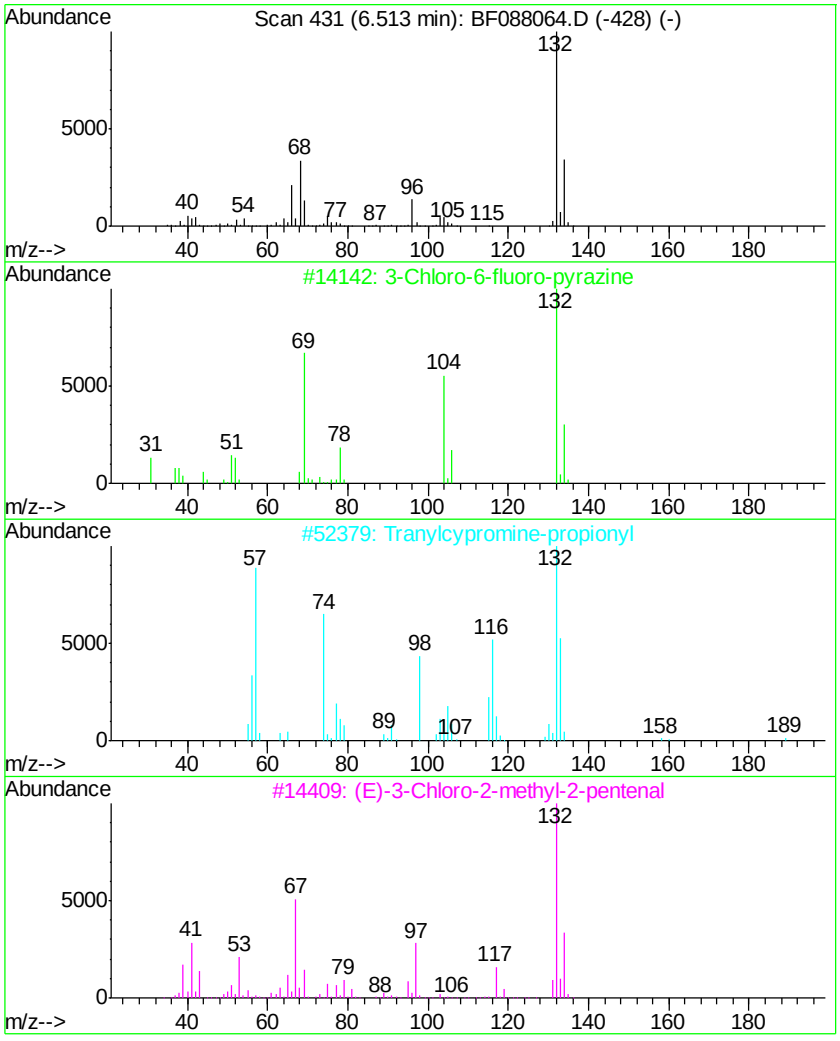
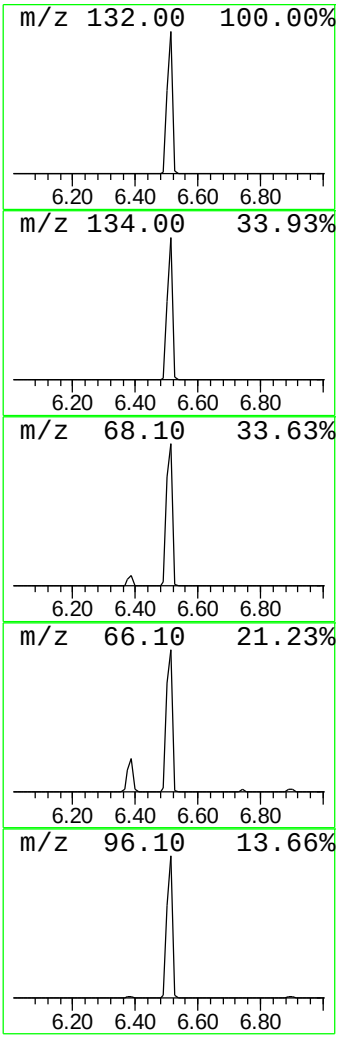
Peak Number 5 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	71.63 ng	2151080	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	38
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : H3570-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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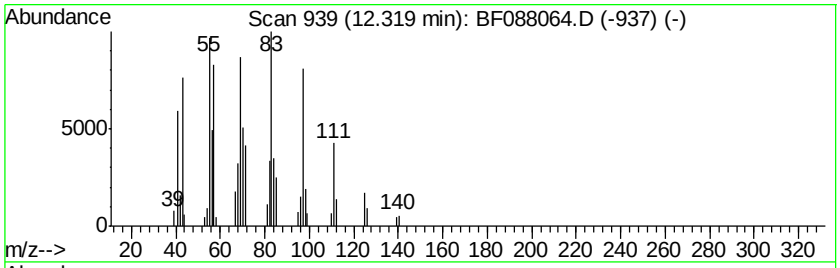
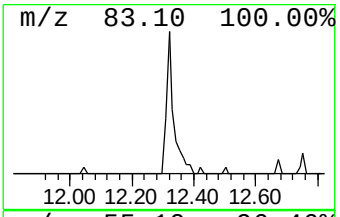
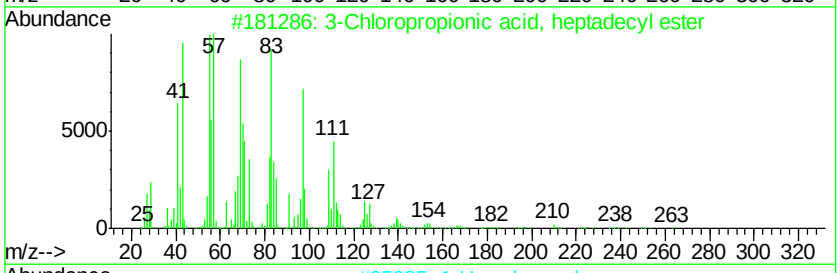
Peak Number 7 3-Chloropropionic acid, hep... Concentration Rank 7

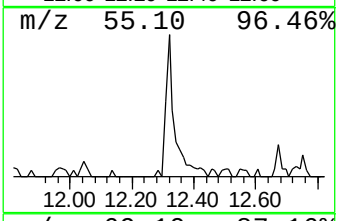
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	3.73 ng	127082	Phenanthrene-d10	11.26

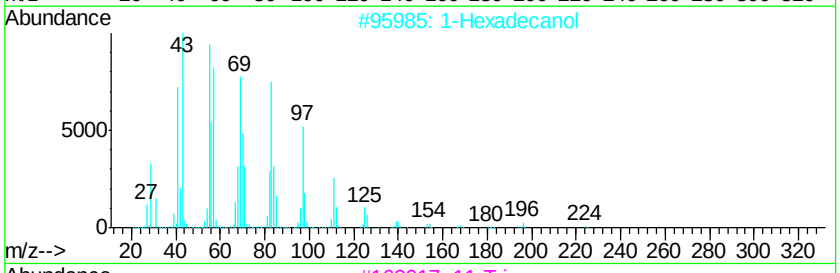
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	91

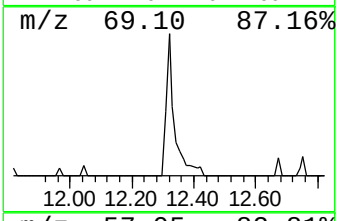


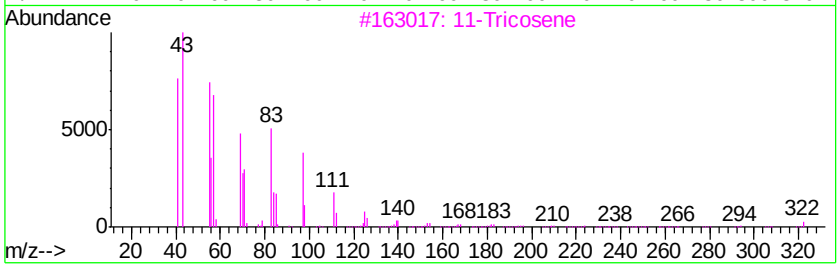


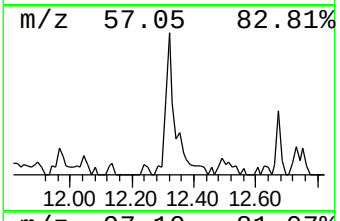


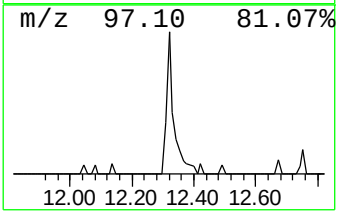












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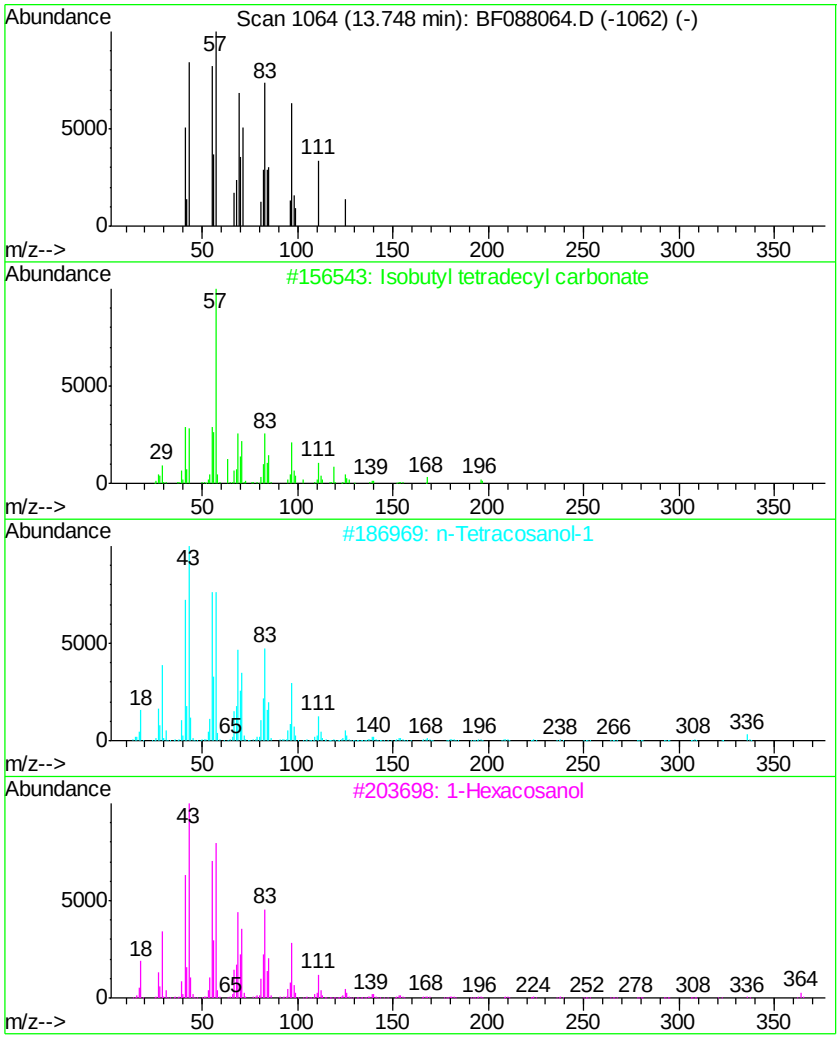
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

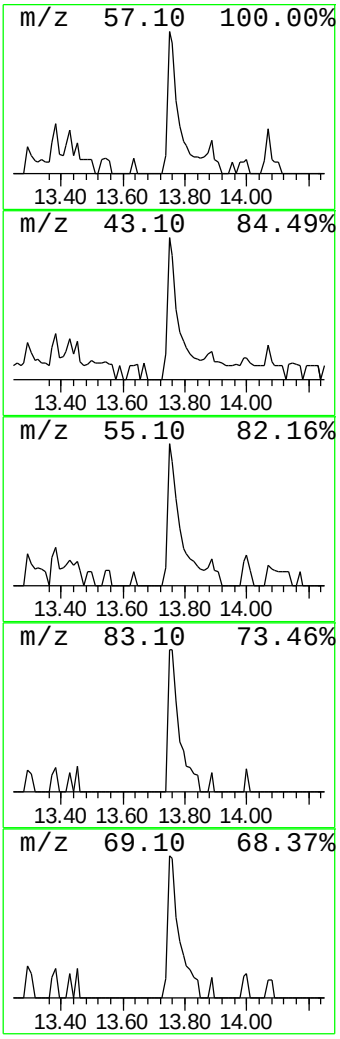
****

Peak Number 8 Isobutyl tetradecyl carbonate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.89 ng	82773	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	68
3	1-Hexacosanol	382	C26H54O	000506-52-5	68
4	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	59
5	1-Eicosanol	298	C20H42O	000629-96-9	59





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.95	12.7	ng	379854	1	6.74	600569	20.0
2-Pentanone, 4-hy...	4.91	4.3	ng	128404	1	6.74	600569	20.0
unknown6.51	6.51	71.6	ng	2151080	1	6.74	600569	20.0
3-Chloropropionic...	12.32	3.7	ng	127082	4	11.26	682168	20.0
Isobutyl tetradec...	13.75	2.9	ng	82773	5	13.89	573345	20.0