LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117817.D
Acq On : 15 Nov 2019 21:47
Operator : JU
Sample : K5861-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

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-BF111319.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	2.187	12	17	27	rVB	647040	852562	18.08%	1.987%
2	5.128	509	517	524	rBV	793311	889067	18.85%	2.072%
3	5.528	580	585	588	rBV	3913153	3487861	73.96%	8.129%
4	6.534	751	756	762	rBV	4009380	3753713	79.59%	8.748%
5	6.687	777	782	785	rBV	4050244	3795236	80.47%	8.845%
6	6.916	818	821	825	rBV	1610644	1373929	29.13%	3.202%
7	7.075	844	848	851	rBV	3695227	3022887	64.10%	7.045%
8	7.475	912	916	920	rBV	2505440	2291505	48.59%	5.341%
9	8.204	1036	1040	1044	rBV	2215337	1791606	37.99%	4.176%
10	9.287	1219	1224	1227	rBV	4699601	4484533	95.09%	10.452%
11	9.675	1286	1290	1294	rBV	488859	375925	7.97%	0.876%
12	9.969	1336	1340	1343	rBV	2429264	2090420	44.32%	4.872%
13	10.757	1470	1474	1477	rBV	3207984	2804345	59.46%	6.536%
14	11.457	1589	1593	1597	rBV	2493252	2187893	46.39%	5.099%
15	11.980	1679	1682	1686	rBV	69958	79669	1.69%	0.186%
16	13.051	1859	1864	1867	rBV	4949528	4716140	100.00%	10.992%
17	13.957	2013	2018	2038	rBV2	138197	447217	9.48%	1.042%
18	14.104	2039	2043	2047	rBV	2032854	1781747	37.78%	4.153%
19	14.269	2067	2071	2075	rBV	84046	77740	1.65%	0.181%
20	14.574	2120	2123	2127	rBV	97856	87344	1.85%	0.204%
21	14.898	2174	2178	2183	rVB	102885	105901	2.25%	0.247%
22	14.974	2187	2191	2196	rBV	268445	288411	6.12%	0.672%
23	15.251	2234	2238	2243	rVB	90991	105094	2.23%	0.245%
24	15.616	2294	2300	2304	rBV	1411854	1785812	37.87%	4.162%
25	15.651	2304	2306	2314	rVB	76803	102129	2.17%	0.238%
26	16.110	2379	2384	2391	rBV2	51673	79555	1.69%	0.185%
27	16.645	2471	2475	2483	rVB2	28000	48770	1.03%	0.114%

Sum of corrected areas: 42907011

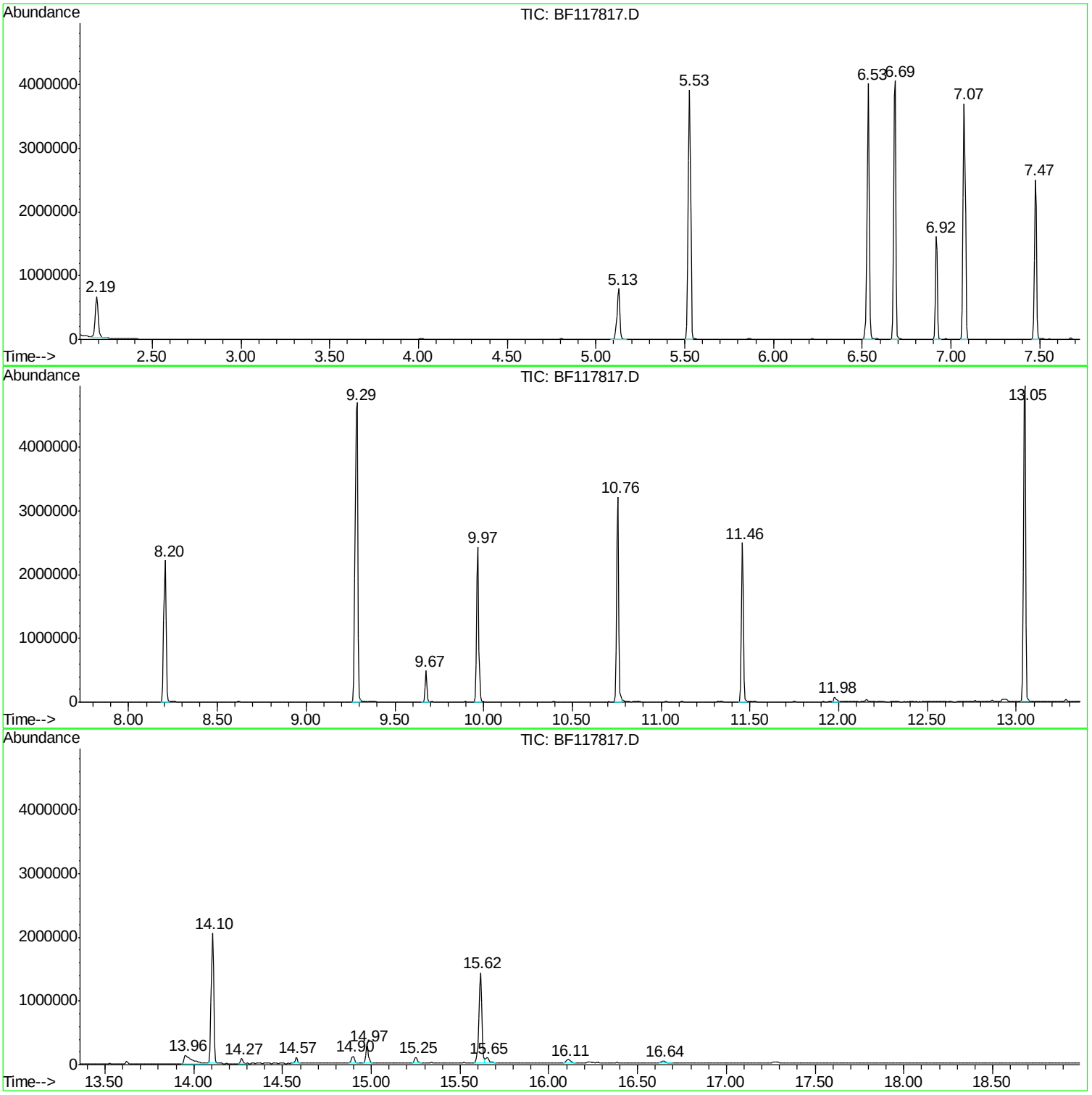
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117817.D
Acq On : 15 Nov 2019 21:47
Operator : JU
Sample : K5861-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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

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Data File : BF117817.D
Acq On : 15 Nov 2019 21:47
Operator : JU
Sample : K5861-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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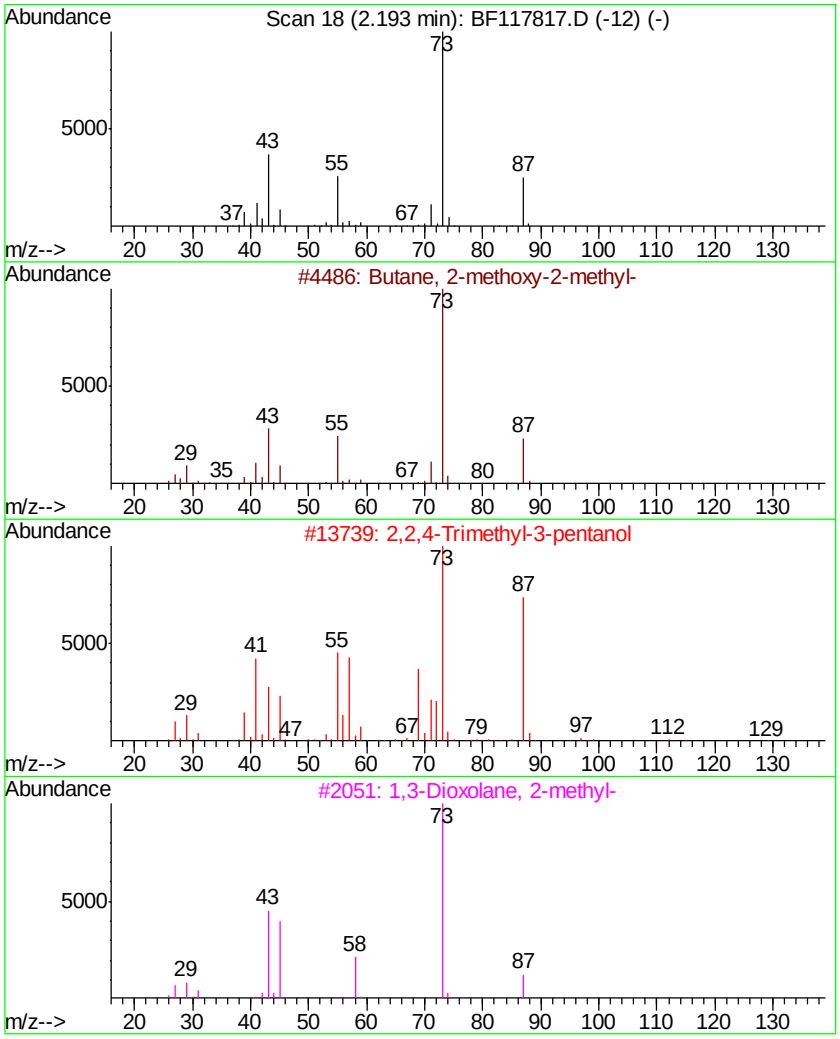
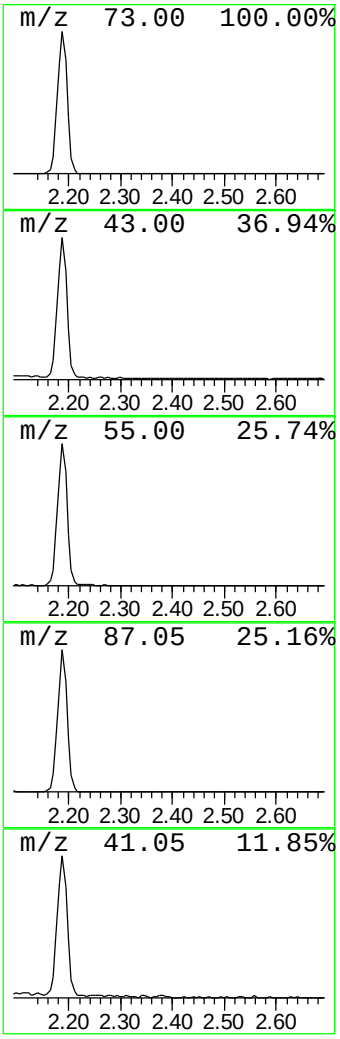
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	12.41 ng	852562	1,4-Dichlorobenzene-d4	6.92

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

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Acq On : 15 Nov 2019 21:47
Operator : JU
Sample : K5861-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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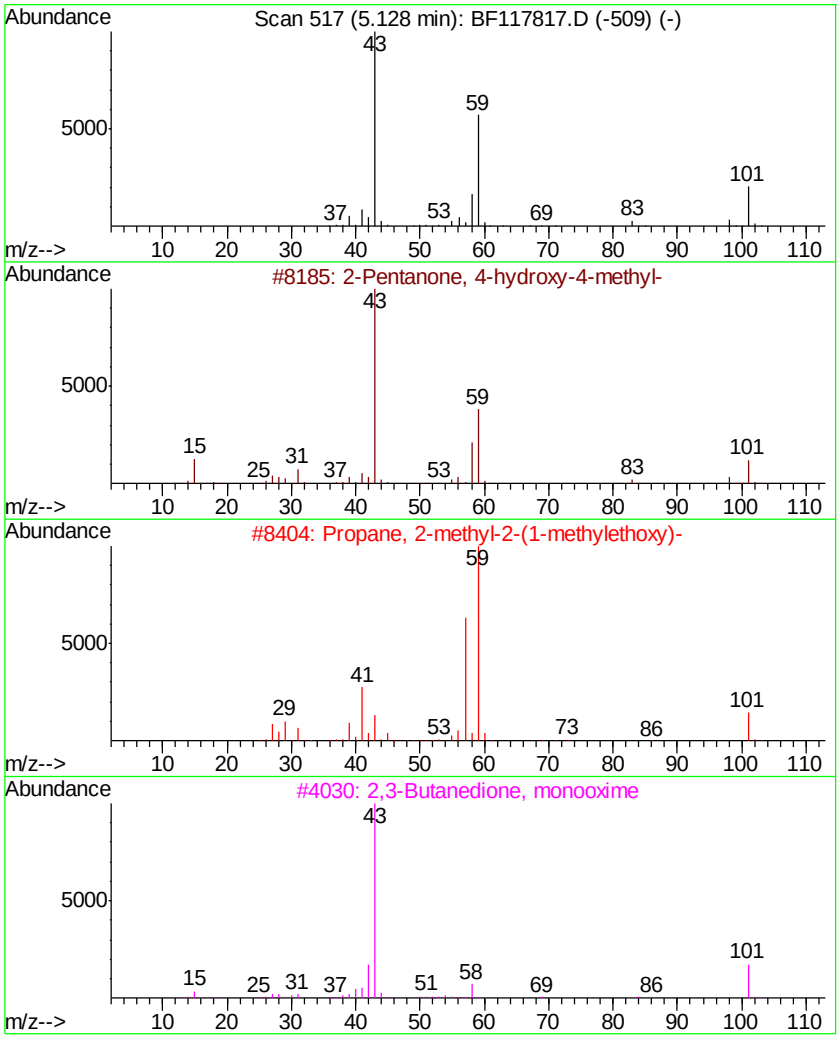
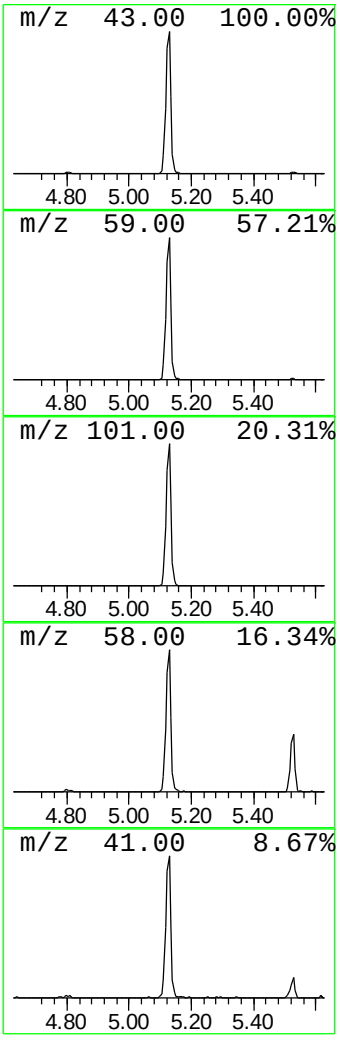
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	12.94 ng	889067	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111519\
Data File : BF117817.D
Acq On : 15 Nov 2019 21:47
Operator : JU
Sample : K5861-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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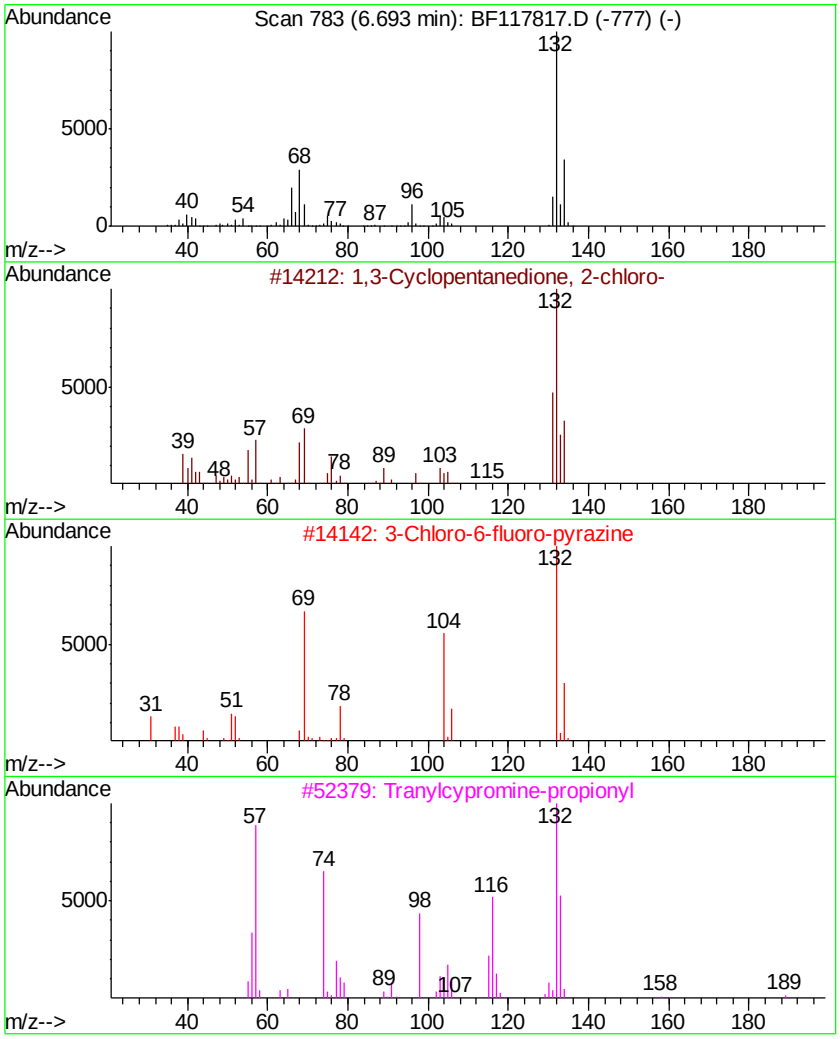
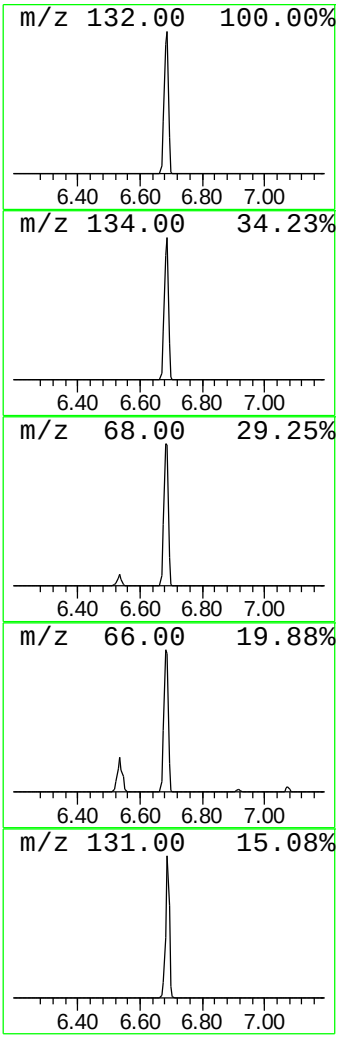
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	55.25 ng	3795240	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	37
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF117817.D
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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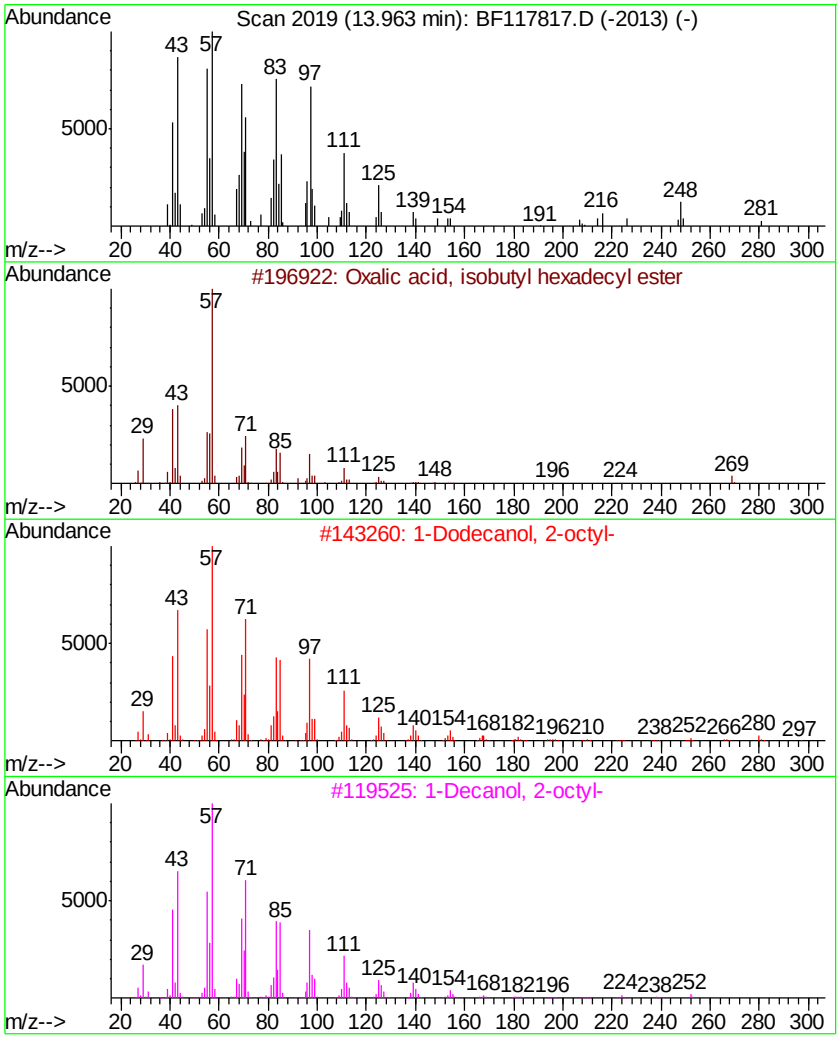
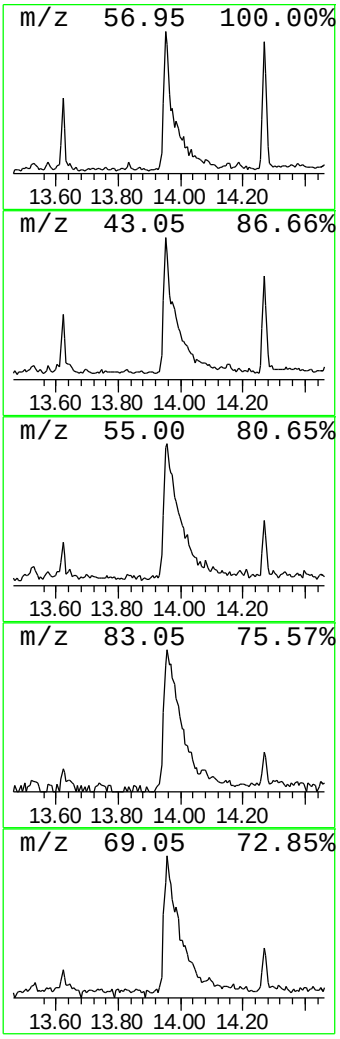
Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.02 ng	447217	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	87
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81





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Sample : K5861-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-16

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

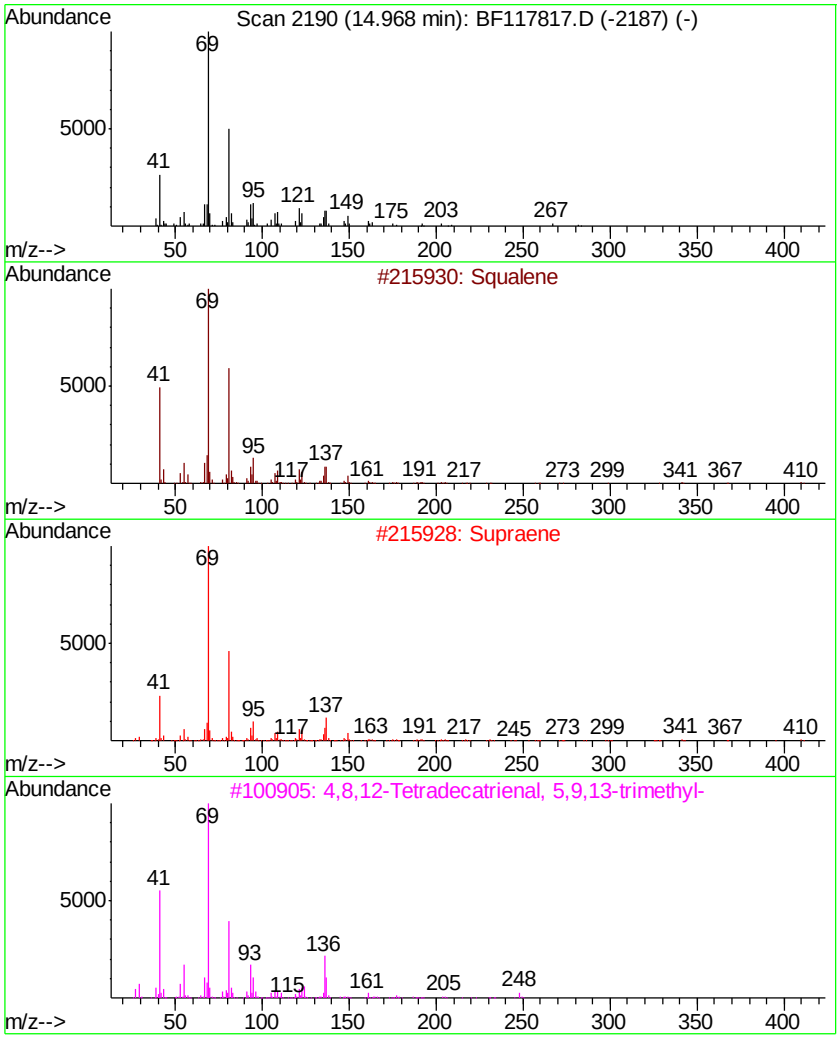
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

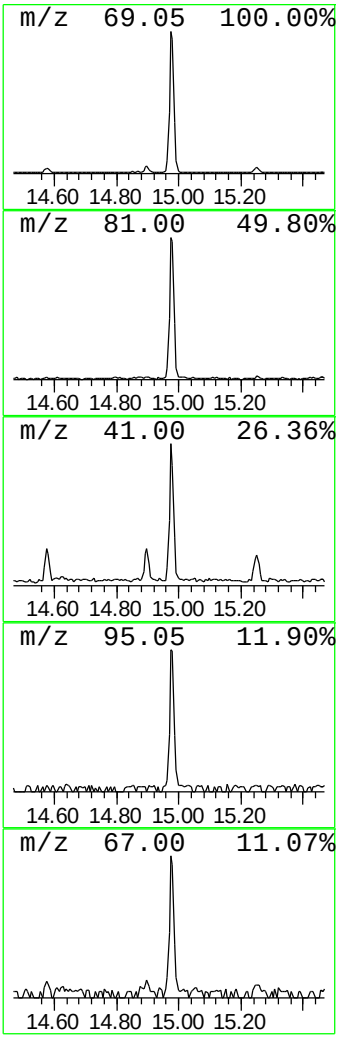
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.23 ng	288411	Perylene-d12	15.62

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	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	50





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	12.4	ng	852562	1	6.92	1373930	20.0
2-Pentanone, 4-hy...	5.13	12.9	ng	889067	1	6.92	1373930	20.0
unknown6.69	6.69	55.3	ng	3795240	1	6.92	1373930	20.0
Oxalic acid, isob...	13.96	5.0	ng	447217	5	14.10	1781750	20.0
Squalene	14.97	3.2	ng	288411	6	15.62	1785810	20.0