LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117866.D
Acq On : 19 Nov 2019 18:20
Operator : JU
Sample : K5904-14
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 12-(2-4)

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	2.222	15	23	30	rVB	869229	1176347	17.72%	2.084%
2	5.140	510	519	527	rBV	793550	1073870	16.18%	1.903%
3	5.534	580	586	589	rBV	5195816	5359514	80.76%	9.497%
4	6.539	751	757	761	rBV	5073538	5984956	90.18%	10.605%
5	6.687	777	782	785	rBV	5953369	5911690	89.08%	10.475%
6	6.734	788	790	804	rVB	83656	95364	1.44%	0.169%
7	6.916	817	821	824	rBV	1618803	1262152	19.02%	2.236%
8	7.075	843	848	851	rBV	5427507	4677097	70.47%	8.287%
9	7.481	911	917	920	rBV	3529379	3691153	55.62%	6.540%
10	8.204	1035	1040	1043	rBV	1735570	1647751	24.83%	2.920%
11	9.280	1218	1223	1226	rBV	6810005	6636734	100.00%	11.760%
12	9.675	1286	1290	1293	rBV	450062	407995	6.15%	0.723%
13	9.963	1335	1339	1343	rBV	2226555	1879840	28.32%	3.331%
14	10.757	1469	1474	1477	rBV	4288972	3836272	57.80%	6.798%
15	10.857	1487	1491	1502	rVB	76001	88599	1.33%	0.157%
16	11.457	1589	1593	1595	rBV	2294705	1843791	27.78%	3.267%
17	11.480	1595	1597	1600	rVV	191176	154112	2.32%	0.273%
18	11.522	1600	1604	1610	rVB3	169731	150670	2.27%	0.267%
19	11.974	1674	1681	1685	rBV4	56077	105140	1.58%	0.186%
20	12.669	1796	1799	1803	rBV	167666	159828	2.41%	0.283%
21	12.904	1834	1839	1843	rVB	136994	144701	2.18%	0.256%
22	13.051	1859	1864	1867	rBV	6131554	6127889	92.33%	10.858%
23	13.963	2013	2019	2035	rBV5	141421	452927	6.82%	0.803%
24	14.104	2035	2043	2046	rBV	1594998	1437091	21.65%	2.546%
25	14.568	2118	2122	2126	rBV	91069	98081	1.48%	0.174%
26	14.886	2172	2176	2182	rBV	116462	129806	1.96%	0.230%
27	15.162	2219	2223	2226	rBV2	47063	72623	1.09%	0.129%
28	15.245	2232	2237	2240	rBV	119366	146149	2.20%	0.259%
29	15.609	2293	2299	2303	rBV	1092753	1366142	20.58%	2.421%
30	15.645	2303	2305	2309	rVB	118111	126716	1.91%	0.225%
31	16.104	2378	2383	2390	rBV	72336	119305	1.80%	0.211%
32	16.639	2469	2474	2479	rBV2	38590	72067	1.09%	0.128%

LSC Area Percent Report

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Acq On : 19 Nov 2019 18:20
Operator : JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-(2-4)

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Integrator: RTE
Smoothing : ON Filtering: 5
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Peak separation: 5

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

Sum of corrected areas: 56436372

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117866.D
Acq On : 19 Nov 2019 18:20
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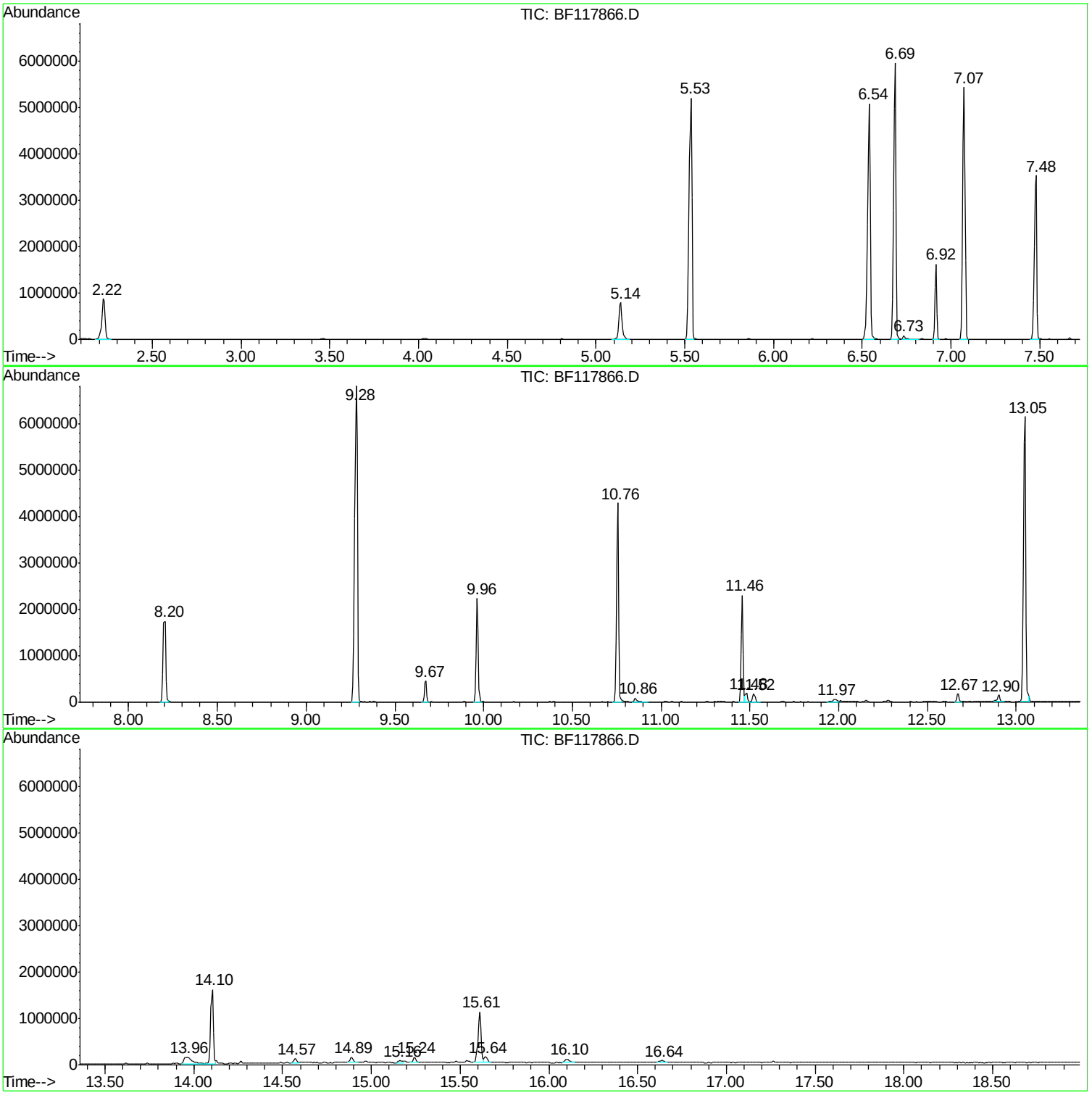
Sample : K5904-14
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-(2-4)

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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Acq On : 19 Nov 2019 18:20
Operator : JU
Sample : K5904-14
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 12-(2-4)

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

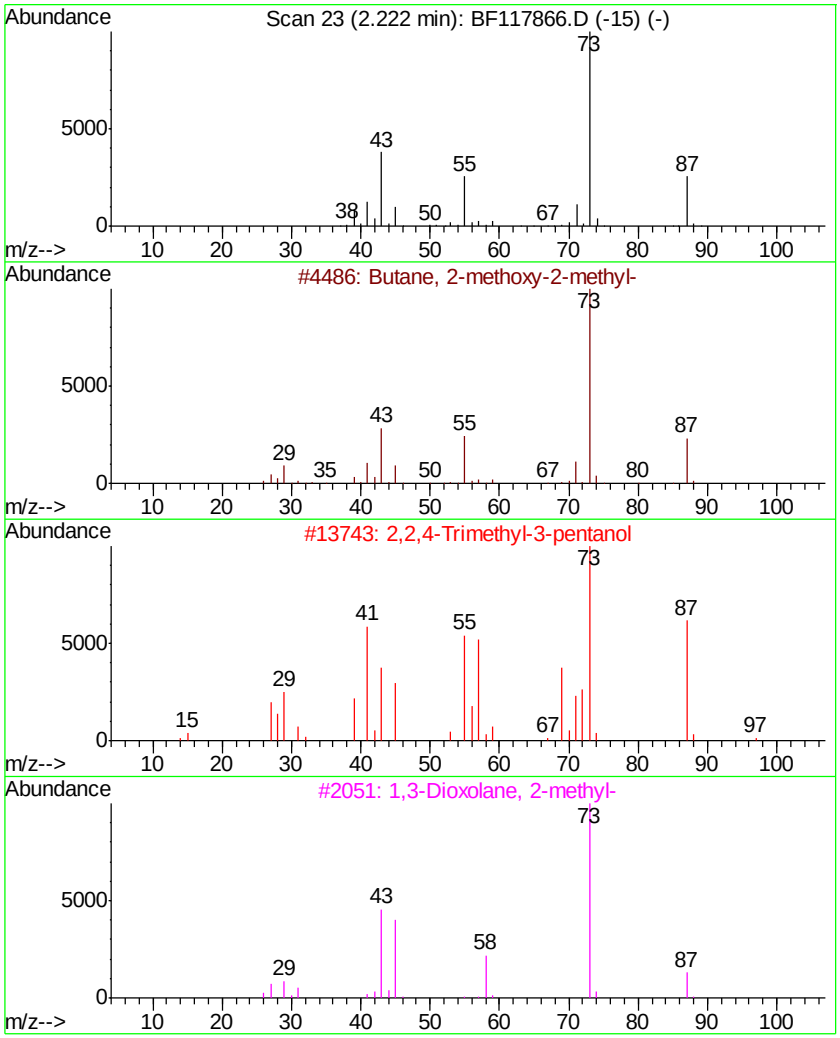
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

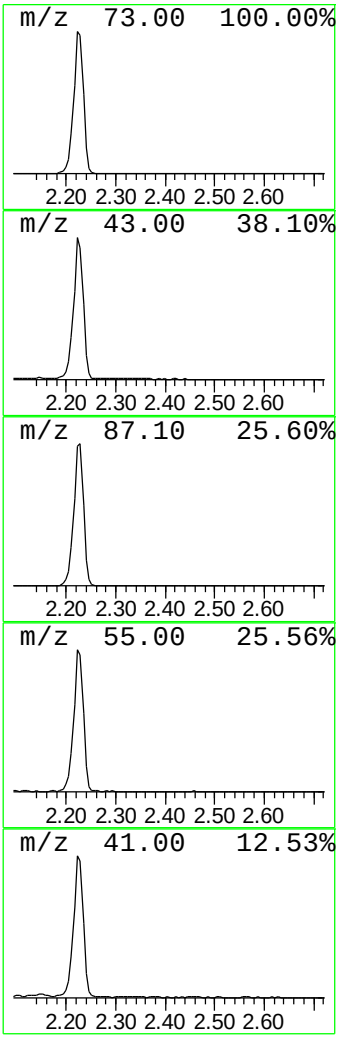
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	18.64 ng	1176350	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	50
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117866.D
Acq On : 19 Nov 2019 18:20
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Sample : K5904-14
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 12-(2-4)

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

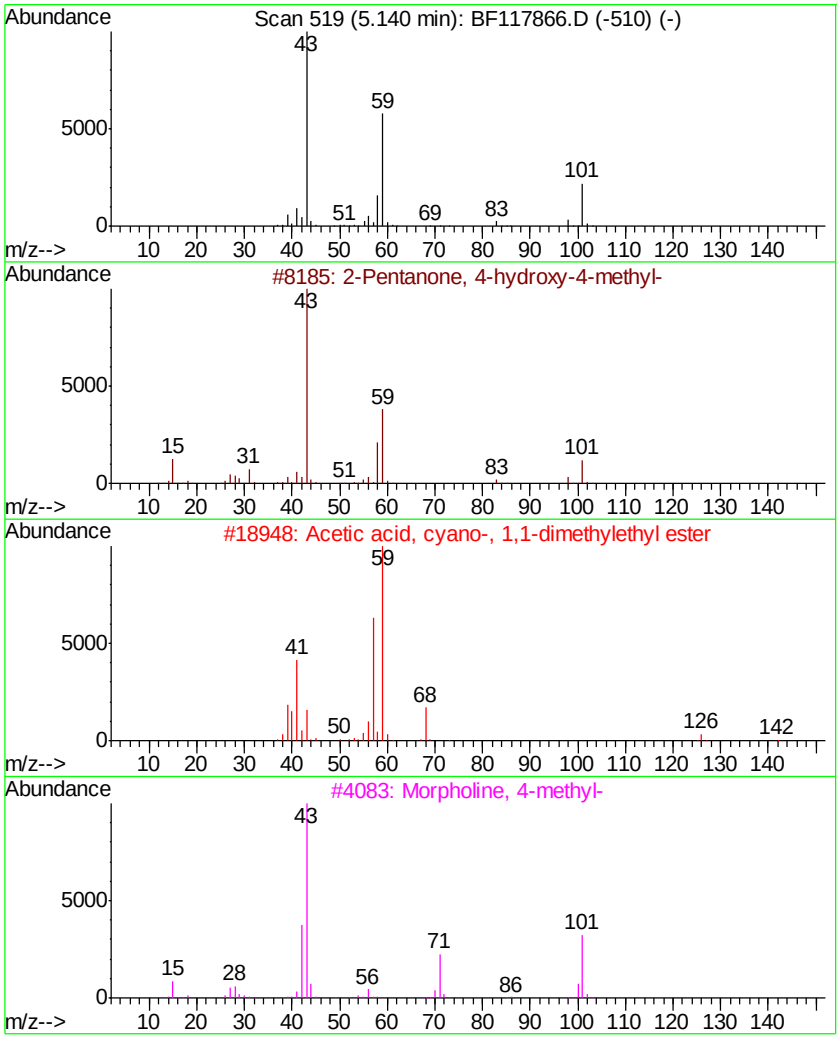
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

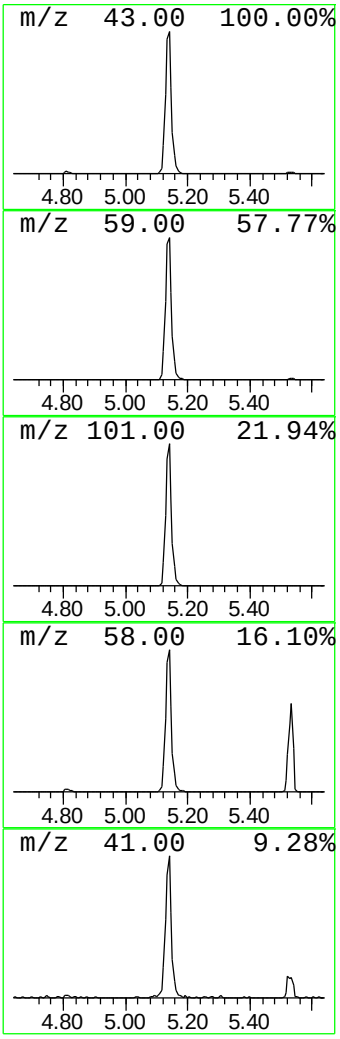
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	17.02 ng	1073870	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	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 12-(2-4)

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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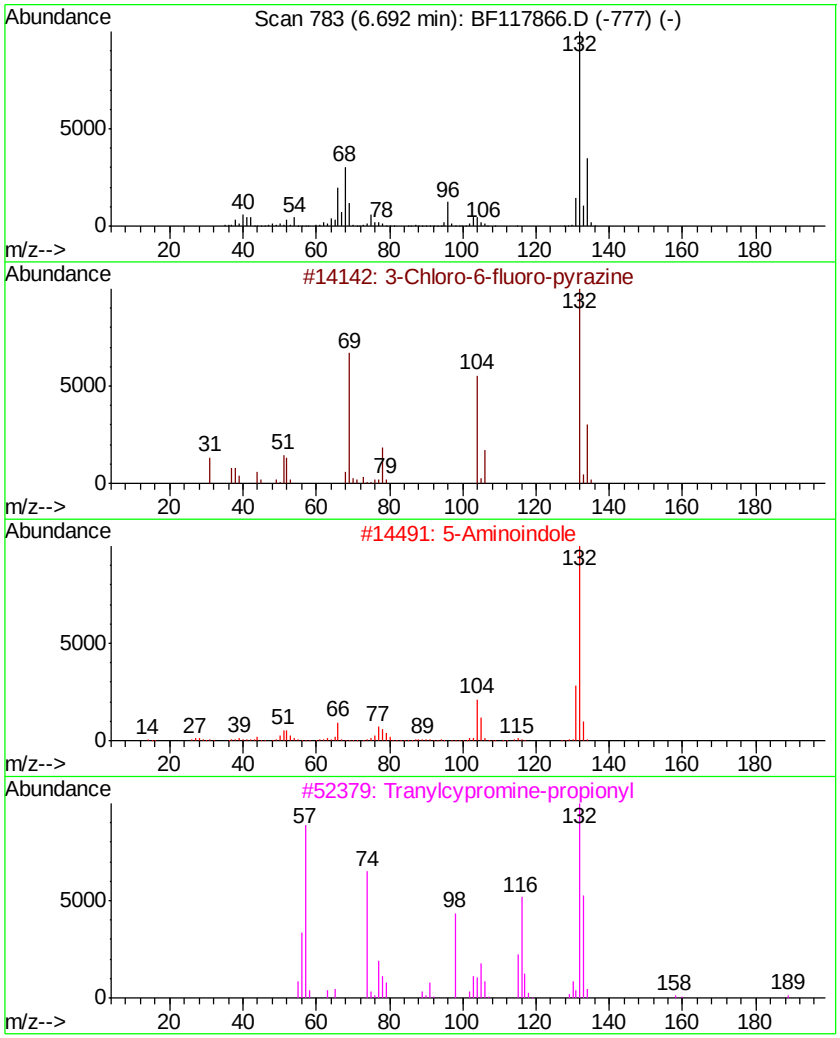
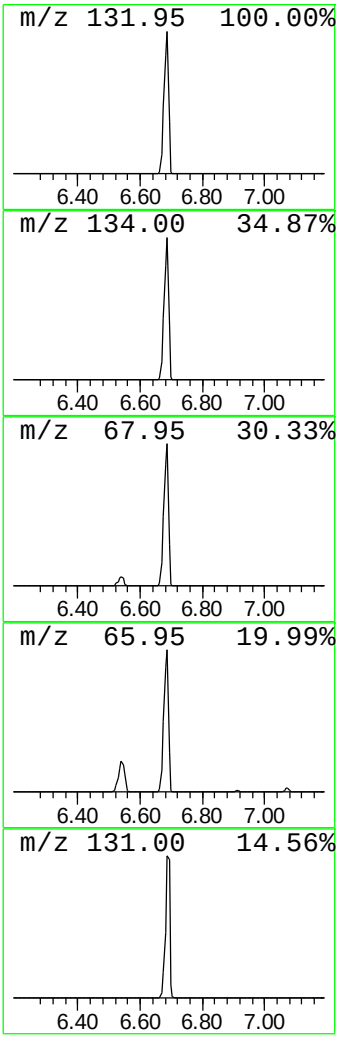
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	93.68 ng	5911690	1,4-Dichlorobenzene-d4	6.92

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	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
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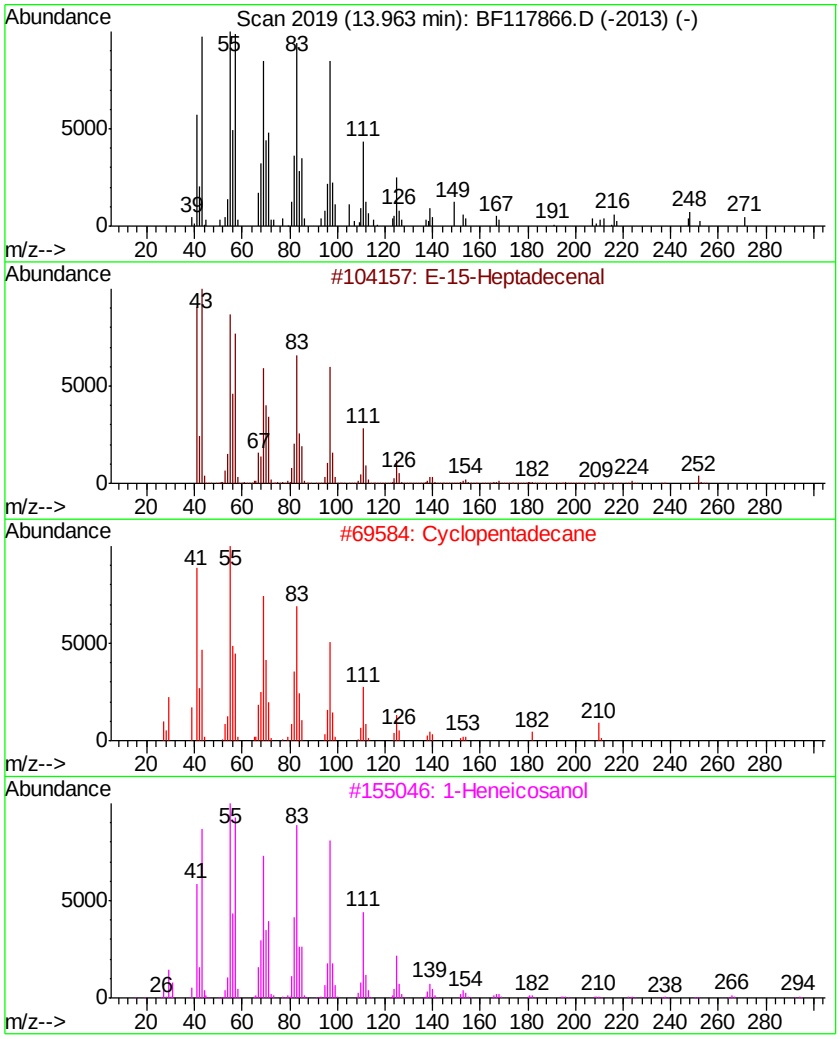
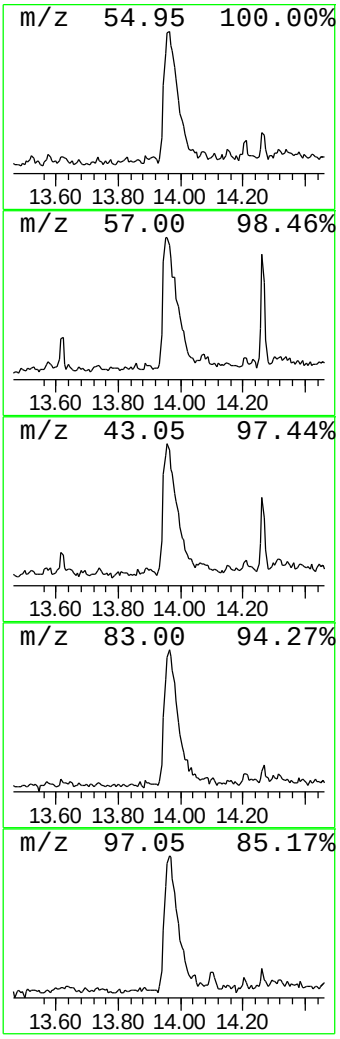
Peak Number 6 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	6.30 ng	452927	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	97
2	Cyclopentadecane	210	C15H30	000295-48-7	96
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95





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Instrument : BNA_F
ClientSampleId : 12-(2-4)

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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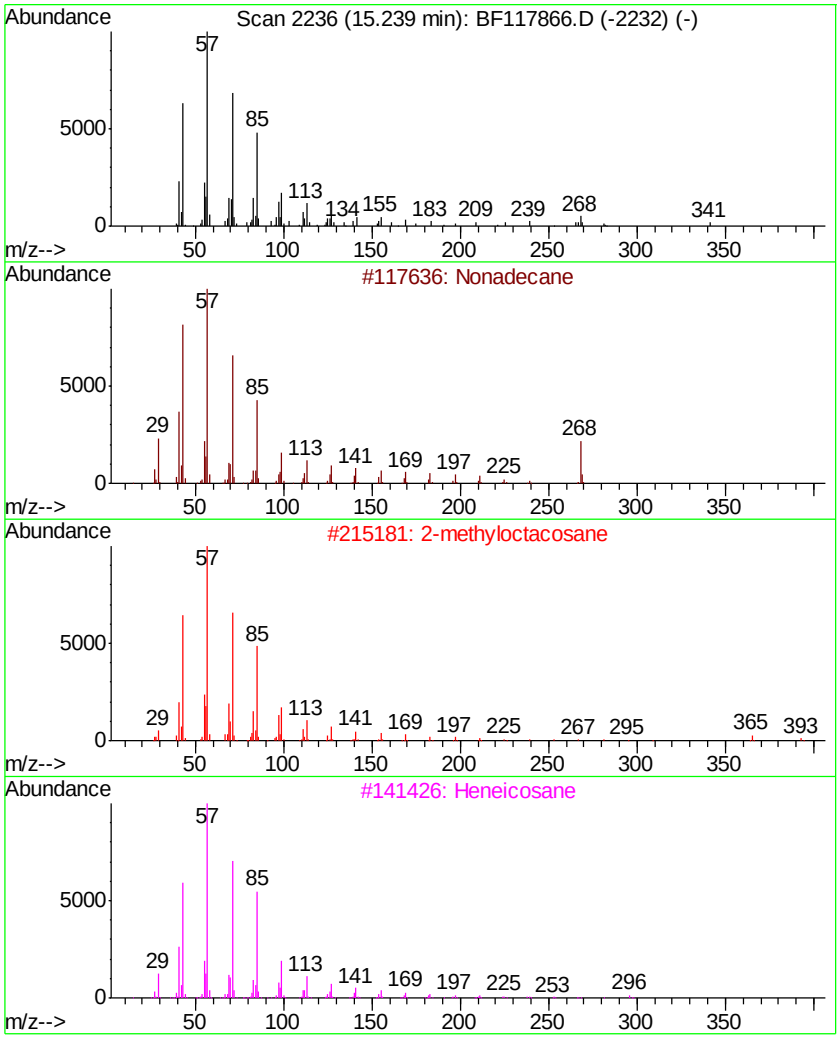
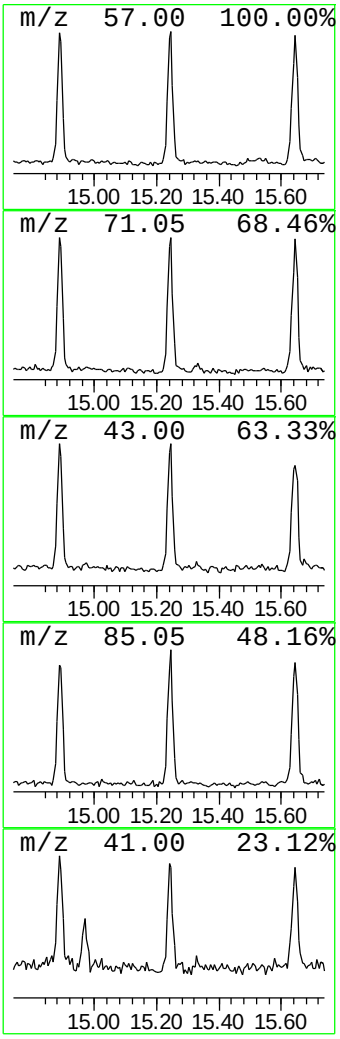
Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.14 ng	146149	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Docosane	310	C22H46	000629-97-0	87





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
Butane, 2-methoxy...	2.22	18.6	ng	1176350	1	6.92	1262150	20.0
2-Pentanone, 4-hy...	5.14	17.0	ng	1073870	1	6.92	1262150	20.0
unknown6.69	6.69	93.7	ng	5911690	1	6.92	1262150	20.0
E-15-Heptadecenal	13.96	6.3	ng	452927	5	14.10	1437090	20.0
Nonadecane	15.24	2.1	ng	146149	6	15.61	1366140	20.0