LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117990.D
Acq On : 26 Nov 2019 2:40
Operator : JU
Sample : K5840-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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	2.158	7	12	21	rVB	371630	493643	23.80%	2.390%
2	5.087	506	510	520	rVB	296663	326159	15.72%	1.579%
3	5.498	576	580	583	rBV	1369805	1216443	58.64%	5.889%
4	6.510	747	752	763	rBV	1705474	1554607	74.94%	7.526%
5	6.657	772	777	780	rBV	1696895	1567776	75.58%	7.590%
6	6.887	813	816	820	rBV	1287143	1071700	51.66%	5.188%
7	7.045	839	843	846	rBV	1697757	1359385	65.53%	6.581%
8	7.451	907	912	915	rBV	1042572	898661	43.32%	4.351%
9	8.175	1031	1035	1039	rBV	1619516	1358114	65.47%	6.575%
10	9.257	1215	1219	1222	rBV	2491330	2074376	100.00%	10.042%
11	9.334	1229	1232	1235	rBV3	27164	32652	1.57%	0.158%
12	9.528	1260	1265	1267	rBV2	38851	44575	2.15%	0.216%
13	9.592	1273	1276	1279	rBV	61627	45685	2.20%	0.221%
14	9.645	1283	1285	1289	rBV	232557	197633	9.53%	0.957%
15	9.939	1331	1335	1338	rBV	1635382	1262796	60.88%	6.113%
16	10.139	1364	1369	1373	rVB3	23671	24585	1.19%	0.119%
17	10.592	1439	1446	1450	rBV6	16446	26990	1.30%	0.131%
18	10.728	1465	1469	1480	rVB	1196481	974010	46.95%	4.715%
19	10.857	1486	1491	1493	rBV4	24515	34576	1.67%	0.167%
20	11.433	1585	1589	1591	rBV	1256635	1137591	54.84%	5.507%
21	11.451	1591	1592	1595	rVB	50270	37484	1.81%	0.181%
22	11.951	1674	1677	1682	rVB2	78884	73139	3.53%	0.354%
23	12.127	1700	1707	1712	rBV	37494	48716	2.35%	0.236%
24	12.645	1793	1795	1801	rBV	89437	79189	3.82%	0.383%
25	12.745	1809	1812	1815	rBV4	25334	31010	1.49%	0.150%
26	12.874	1829	1834	1840	rBV2	74812	98520	4.75%	0.477%
27	13.022	1852	1859	1862	rBV	1793014	1543762	74.42%	7.474%
28	13.251	1893	1898	1900	rVB2	44939	47025	2.27%	0.228%
29	13.592	1952	1956	1960	rBV2	32933	53709	2.59%	0.260%
30	13.921	2009	2012	2024	rBV2	134822	257022	12.39%	1.244%
31	14.080	2035	2039	2042	rBV	969644	924631	44.57%	4.476%
32	14.239	2064	2066	2068	rBV2	29572	26184	1.26%	0.127%
33	14.469	2101	2105	2106	rBV3	42514	47315	2.28%	0.229%
34	14.545	2112	2118	2120	rBV2	84064	113201	5.46%	0.548%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

35	14.863	2169	2172	2175	rVB	42037	37228	1.79%	0.180%
36	14.939	2182	2185	2189	rVB	42602	44411	2.14%	0.215%
37	15.210	2228	2231	2236	rBV	75115	109233	5.27%	0.529%
38	15.580	2289	2294	2297	rBV	739604	954538	46.02%	4.621%
39	15.945	2352	2356	2362	rVB7	58343	87979	4.24%	0.426%
40	16.063	2372	2376	2381	rBV2	48079	69279	3.34%	0.335%
41	16.586	2462	2465	2471	rVB5	43566	84682	4.08%	0.410%
42	16.704	2482	2485	2486	rBV3	31801	33301	1.61%	0.161%
43	16.892	2513	2517	2520	rBV5	37974	73281	3.53%	0.355%
44	17.509	2619	2622	2623	rBV3	21058	26366	1.27%	0.128%
45	17.692	2649	2653	2655	rBV5	33017	52988	2.55%	0.257%

Sum of corrected areas: 20656150

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
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Operator : JU
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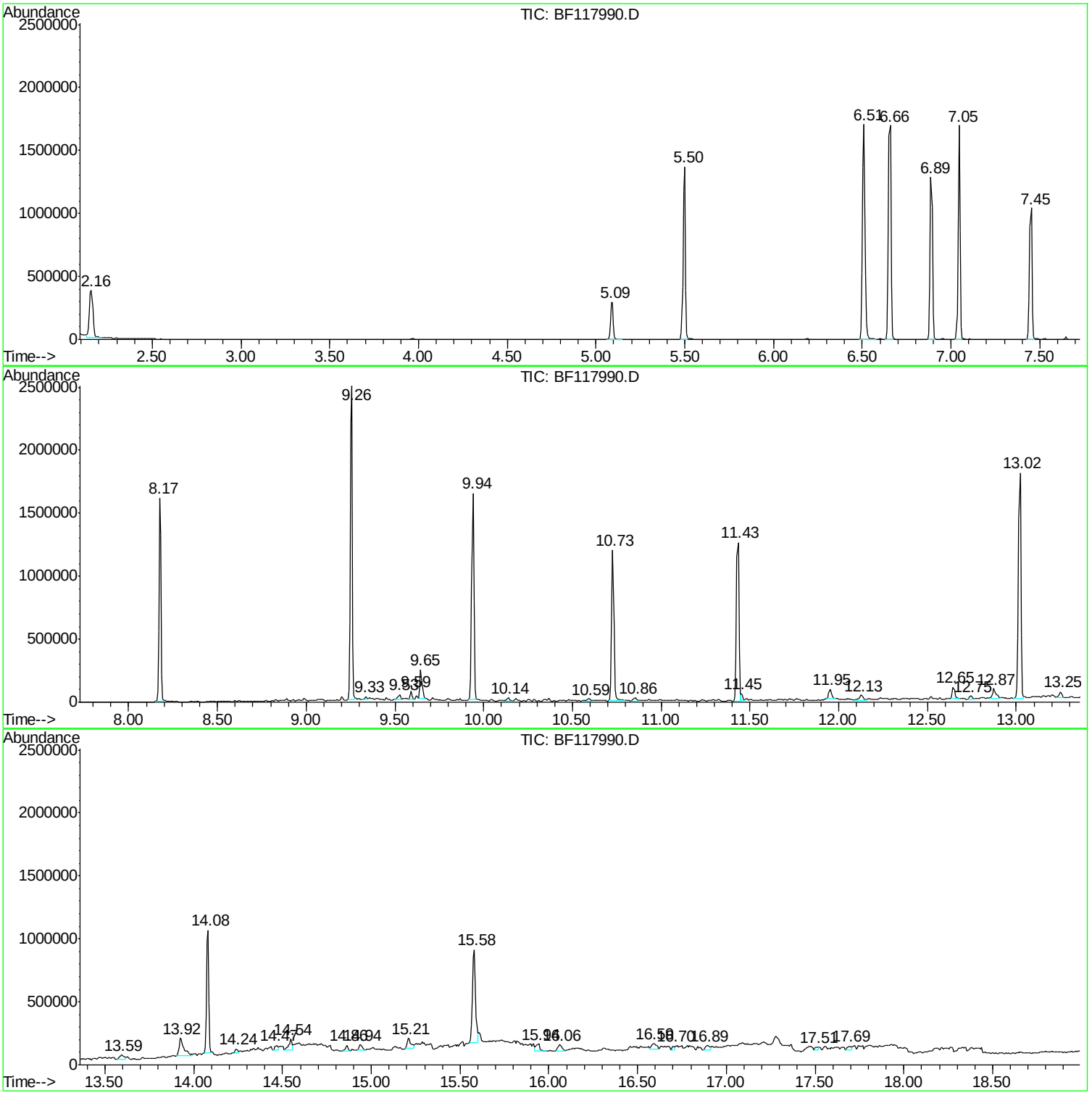
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117990.D
Acq On : 26 Nov 2019 2:40
Operator : JU
Sample : K5840-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

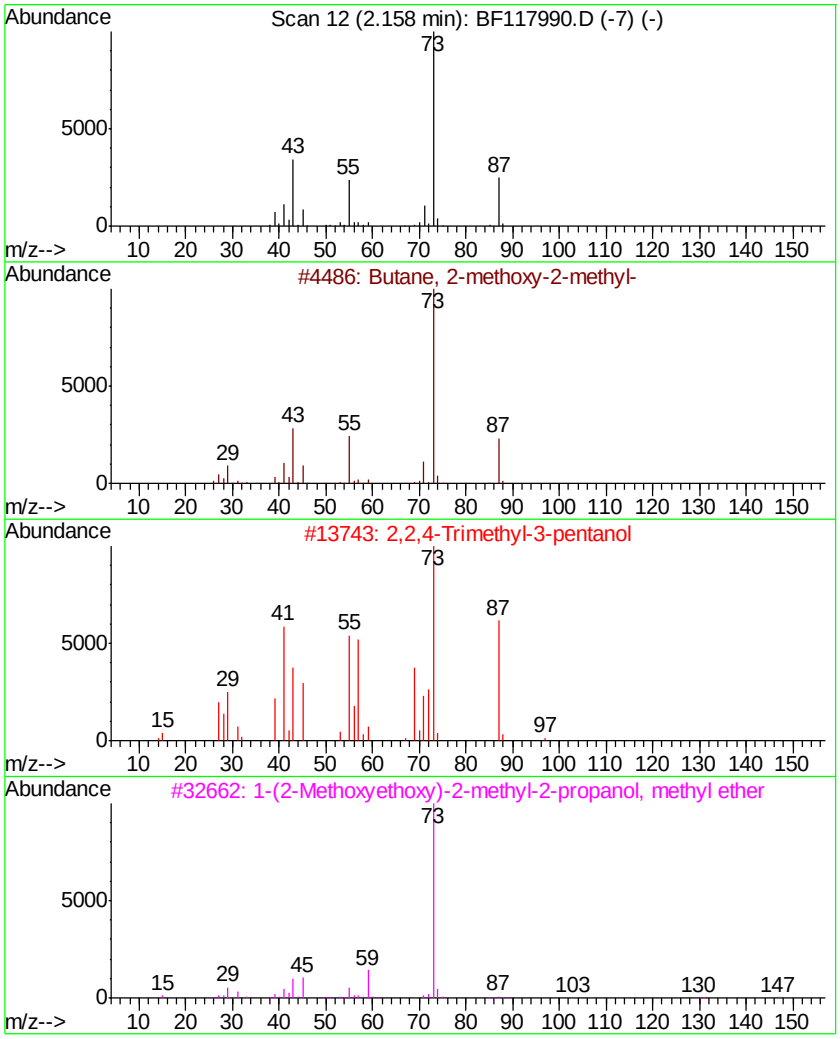
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

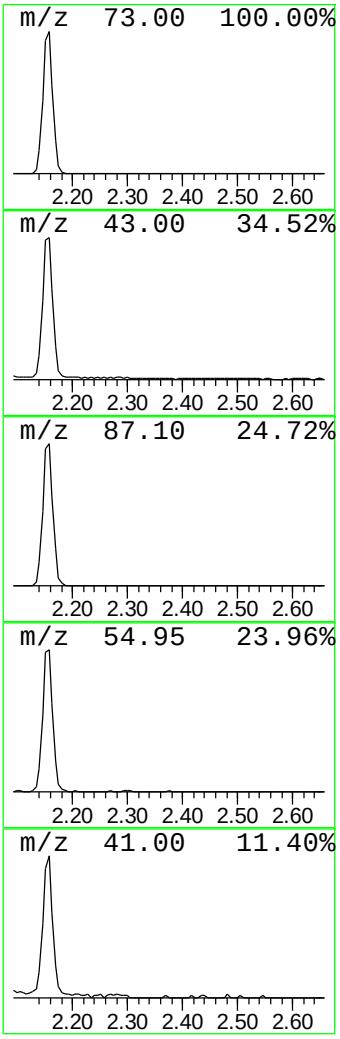
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.21 ng	493643	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117990.D
Acq On : 26 Nov 2019 2:40
Operator : JU
Sample : K5840-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

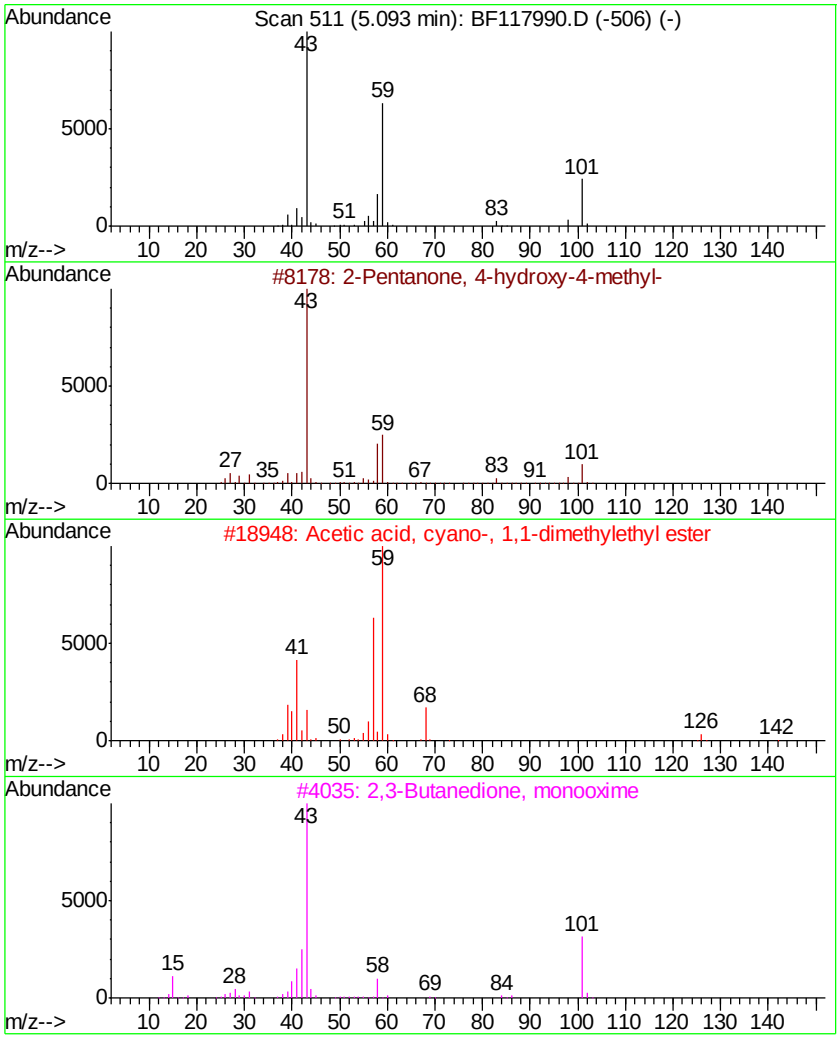
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

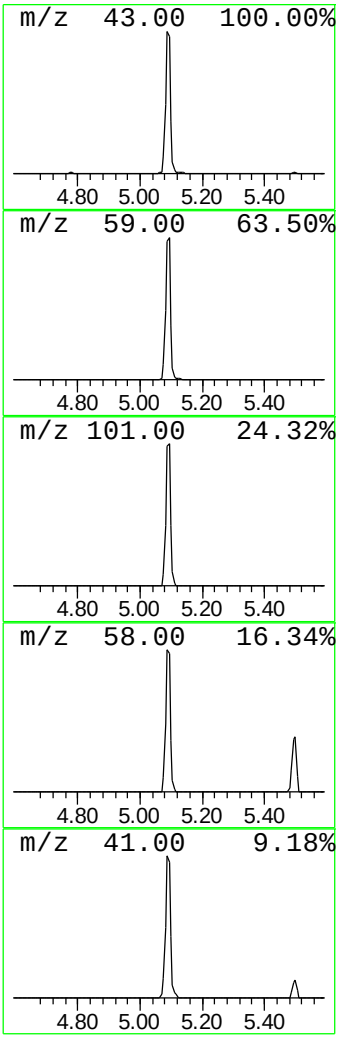
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.09 ng	326159	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Operator : JU
Sample : K5840-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

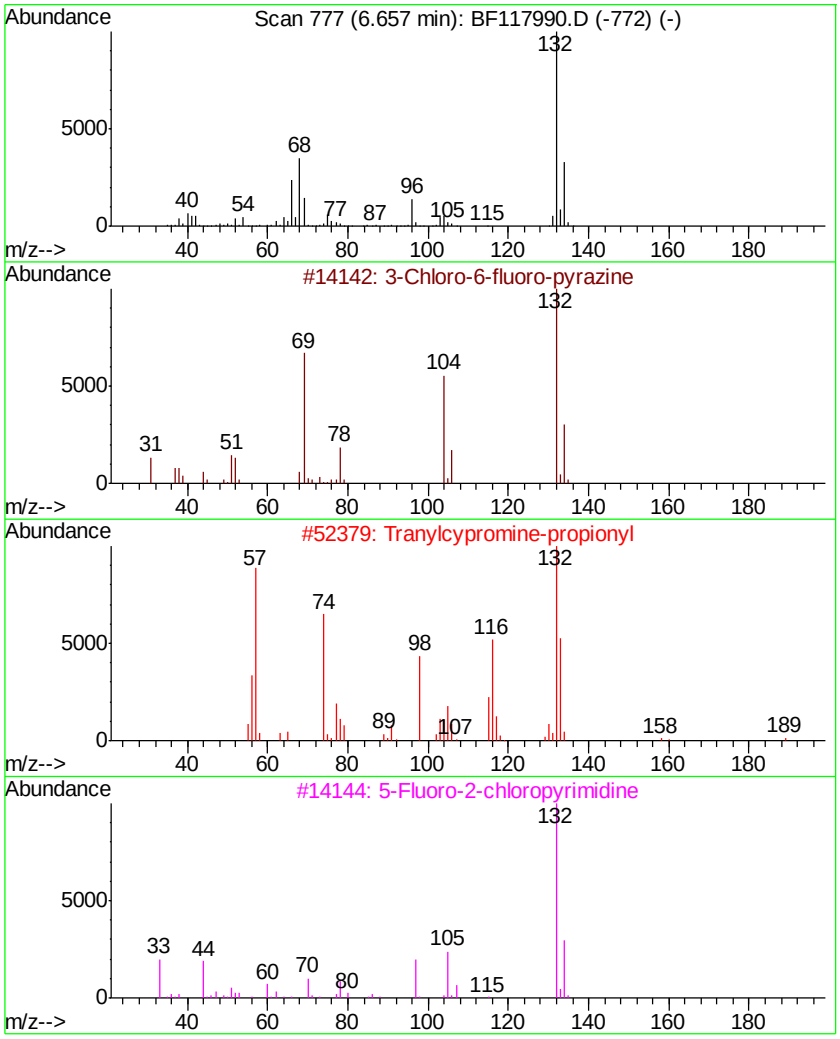
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

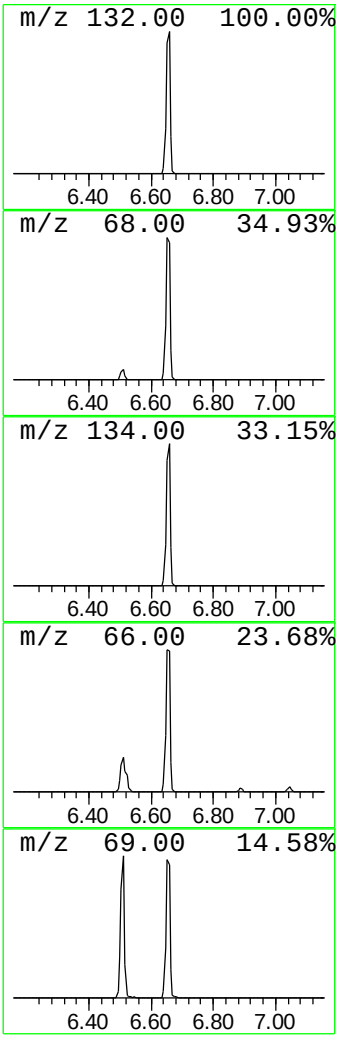
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	29.26 ng	1567780	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
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Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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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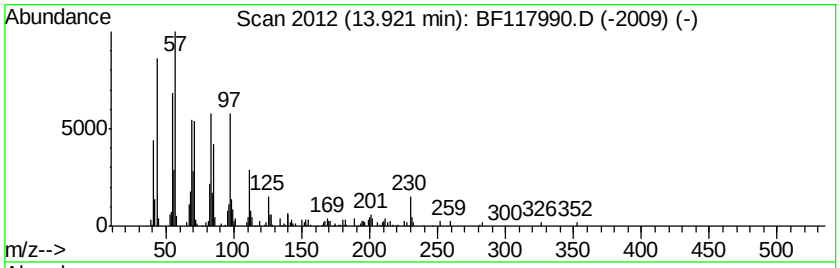
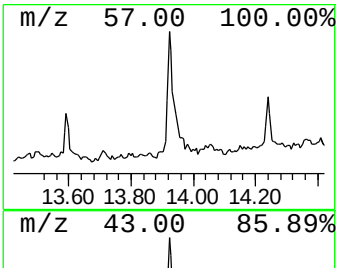
Peak Number 6 Docosyl pentafluoropropionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	5.56 ng	257022	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	94
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91





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Misc :
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Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

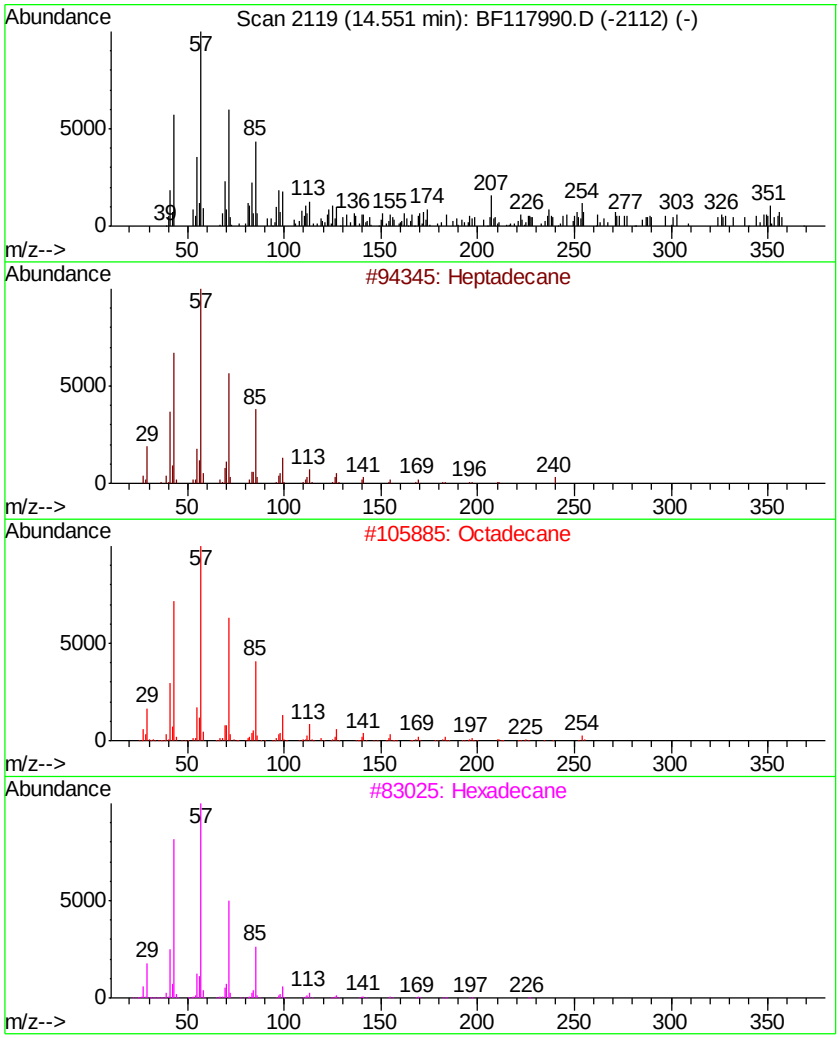
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

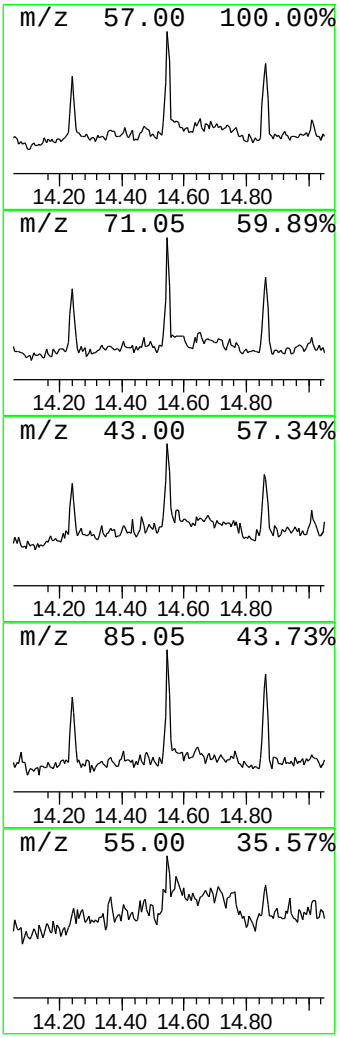
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.45 ng	113201	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Octadecane	254	C18H38	000593-45-3	96
3	Hexadecane	226	C16H34	000544-76-3	94
4	Hexacosane	366	C26H54	000630-01-3	94
5	Pentacosane	352	C25H52	000629-99-2	93





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ClientSampleId : PHIPPS-BH-NE-01

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

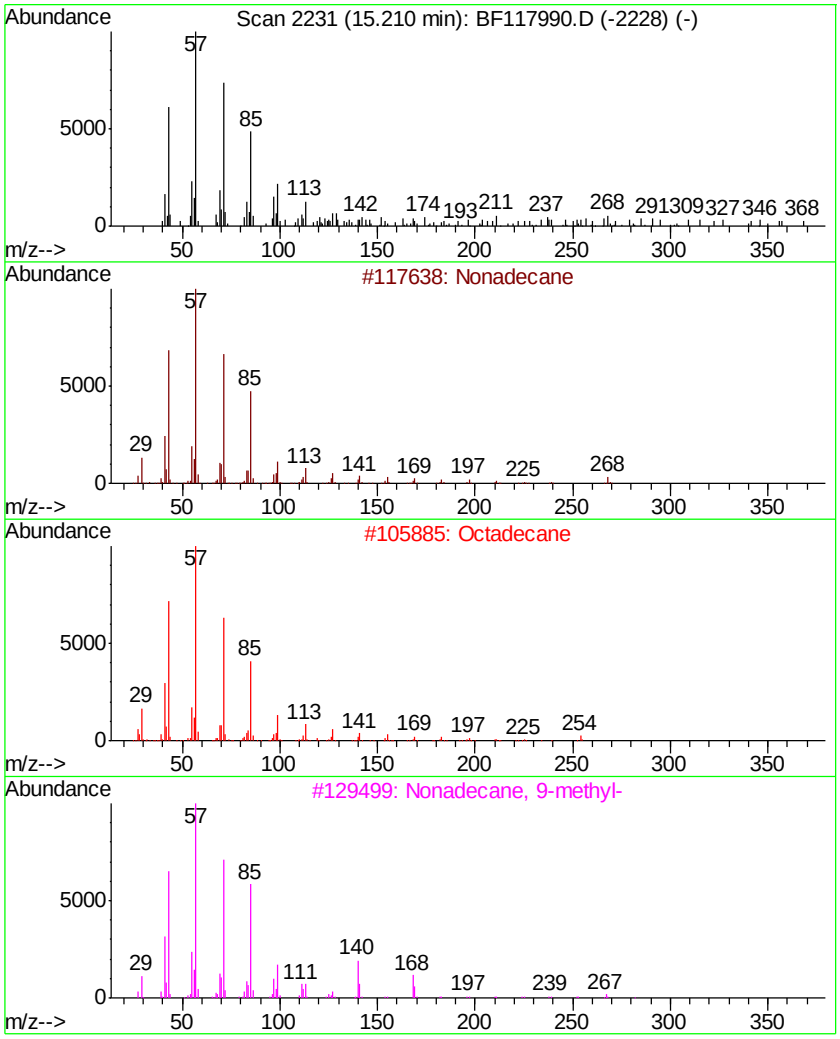
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

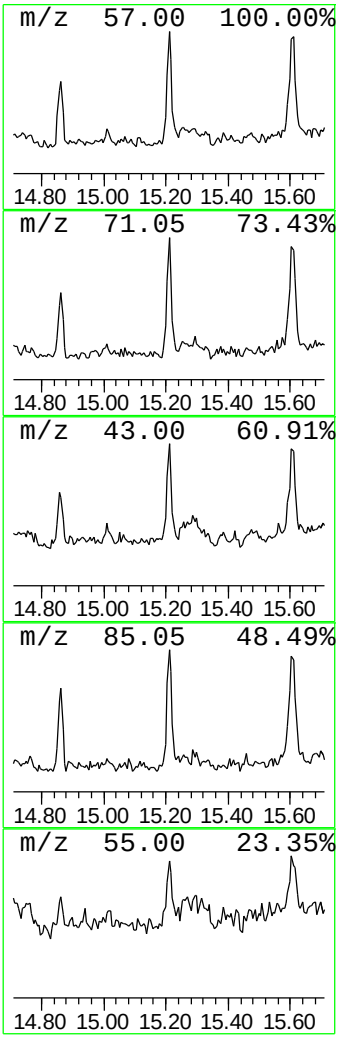
****

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.29 ng	109233	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Octadecane	254	C18H38	000593-45-3	93
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	89
4	Hexacosane	366	C26H54	000630-01-3	83
5	Triacontane	422	C30H62	000638-68-6	72





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : PHIPPS-BH-NE-01

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	9.2	ng	493643	1	6.89	1071700	20.0
2-Pentanone, 4-hy...	5.09	6.1	ng	326159	1	6.89	1071700	20.0
unknown6.66	6.66	29.3	ng	1567780	1	6.89	1071700	20.0
Docosyl pentafluo...	13.92	5.6	ng	257022	5	14.08	924631	20.0
Heptadecane	14.55	2.5	ng	113201	5	14.08	924631	20.0
Nonadecane	15.21	2.3	ng	109233	6	15.58	954538	20.0