LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA N\DATA\BN030618\
Data File : BN000264.D
Acq On : 06 Mar 2018 15:24
Operator : JU/SJ
Sample : J1699-45
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : B14

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_N\METHODS\8270-BN020718.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	3.228	36	41	51	rBV2	96051	236439	2.55%	0.340%
2	3.311	51	55	68	rVB	145158	242092	2.61%	0.348%
3	5.434	410	416	428	rVB2	59843	98504	1.06%	0.141%
4	5.928	492	500	512	rBV	2635193	4284319	46.27%	6.153%
5	7.575	772	780	793	rBV	2996625	4888178	52.79%	7.020%
6	7.969	836	847	867	rBV	2875417	4919537	53.13%	7.065%
7	8.446	922	928	941	rVB	906910	1545334	16.69%	2.219%
8	8.775	977	984	994	rVB	2074279	3582368	38.69%	5.145%
9	9.628	1120	1129	1137	rBV	1792151	2999700	32.40%	4.308%
10	11.287	1403	1411	1419	rBV	1442351	2470770	26.69%	3.548%
11	13.422	1768	1774	1787	rBV	120144	193987	2.10%	0.279%
12	13.687	1809	1819	1833	rBV	4895319	7539933	81.43%	10.828%
13	13.969	1862	1867	1876	rVB	168560	259199	2.80%	0.372%
14	14.563	1963	1968	1975	rVB3	76426	98416	1.06%	0.141%
15	15.057	2045	2052	2061	rVB2	2150535	3314407	35.80%	4.760%
16	15.816	2175	2181	2183	rBV	83294	120107	1.30%	0.172%
17	16.204	2243	2247	2253	rBV	139448	184384	1.99%	0.265%
18	16.528	2296	2302	2320	rBV	3332694	4880184	52.71%	7.008%
19	17.781	2508	2515	2520	rBV	2727300	3837835	41.45%	5.511%
20	18.028	2552	2557	2563	rBV	261711	326447	3.53%	0.469%
21	18.398	2616	2620	2628	rVB	167113	212907	2.30%	0.306%
22	18.616	2652	2657	2664	rBV	280487	438031	4.73%	0.629%
23	18.698	2666	2671	2679	rVB	1533883	1854920	20.03%	2.664%
24	19.522	2806	2811	2813	rBV2	304743	394118	4.26%	0.566%
25	19.551	2813	2816	2827	rVB	400046	554189	5.99%	0.796%
26	19.675	2833	2837	2843	rVB2	97439	131893	1.42%	0.189%
27	19.863	2866	2869	2877	rBV3	80171	126428	1.37%	0.182%
28	20.092	2904	2908	2911	rBV	173345	199399	2.15%	0.286%
29	20.339	2944	2950	2956	rVB	7584837	9258931	100.00%	13.297%
30	20.616	2993	2997	3001	rBV	276954	304571	3.29%	0.437%
31	21.098	3076	3079	3083	rBV	273806	303401	3.28%	0.436%
32	21.557	3153	3157	3175	rVB	428258	591514	6.39%	0.849%
33	21.763	3189	3192	3201	rVB	136050	157460	1.70%	0.226%
34	21.892	3208	3214	3226	rVB2	3191563	4443350	47.99%	6.381%

LSC Area Percent Report

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Misc :
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Instrument : BNA_N
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.004	3229	3233	3238	rVB	124214	163670	1.77%	0.235%
36	24.368	3627	3635	3650	rVB	2163675	4476617	48.35%	6.429%

Sum of corrected areas: 69633539

LSC Report - Integrated Chromatogram

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Data File : BN000264.D
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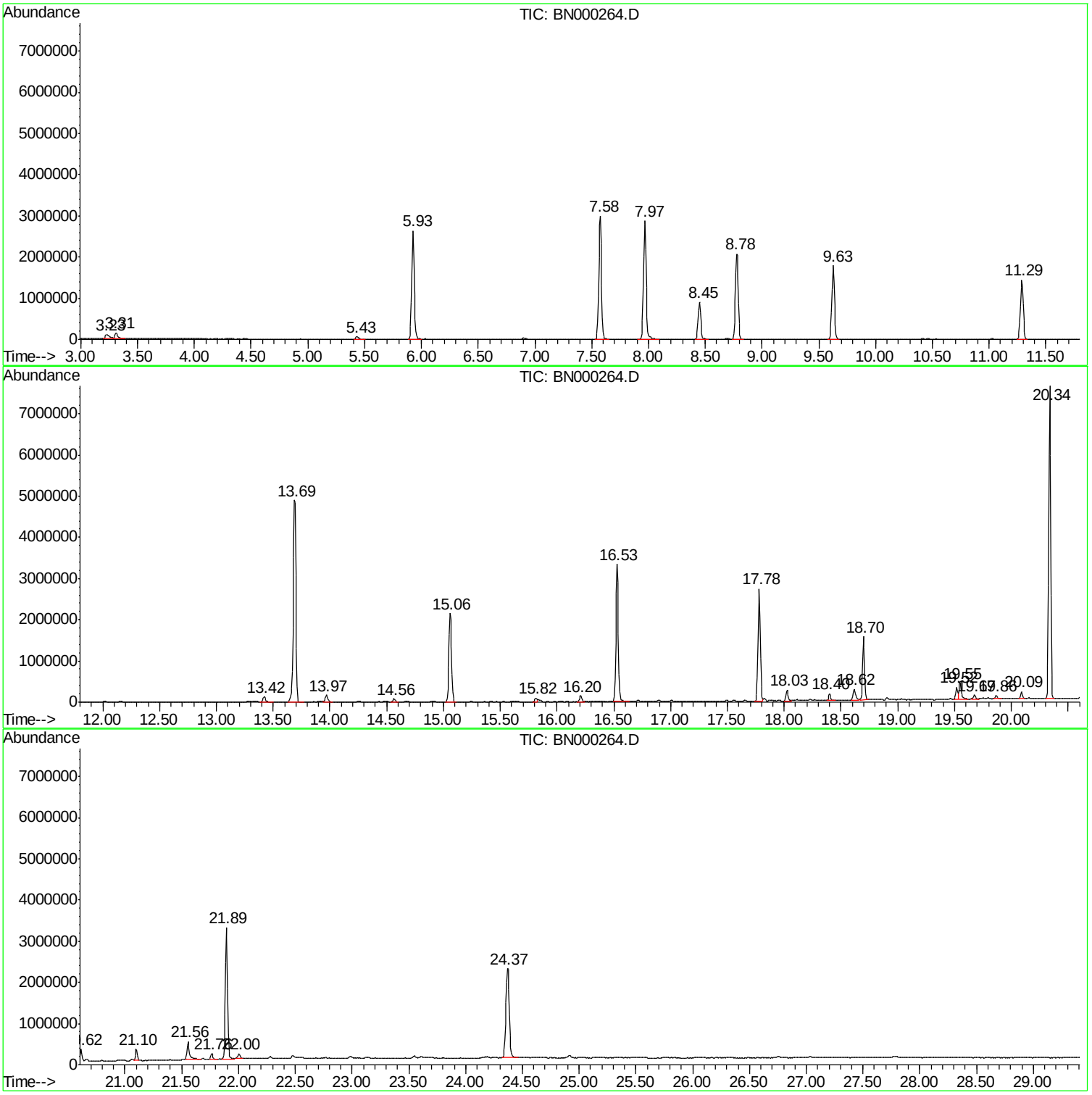
Operator : JU/SJ
Sample : J1699-45
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : B14

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA N\DATA\BN030618\
Data File : BN000264.D
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Sample : J1699-45
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : B14

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

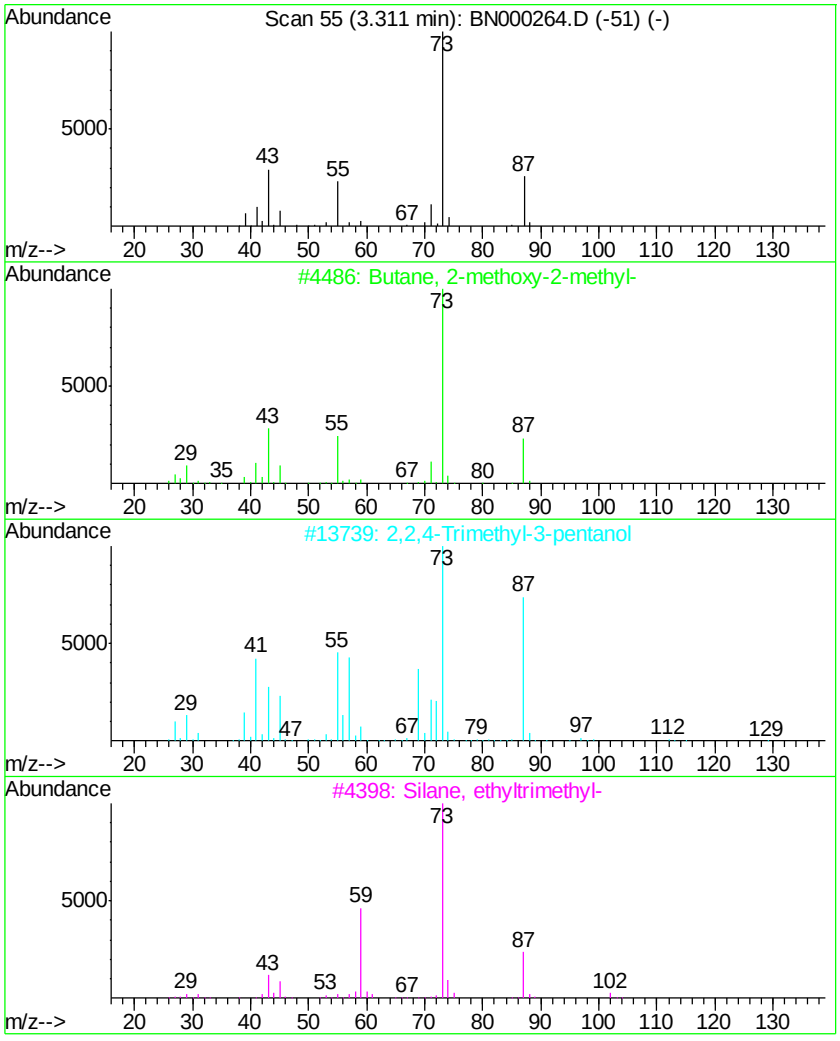
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

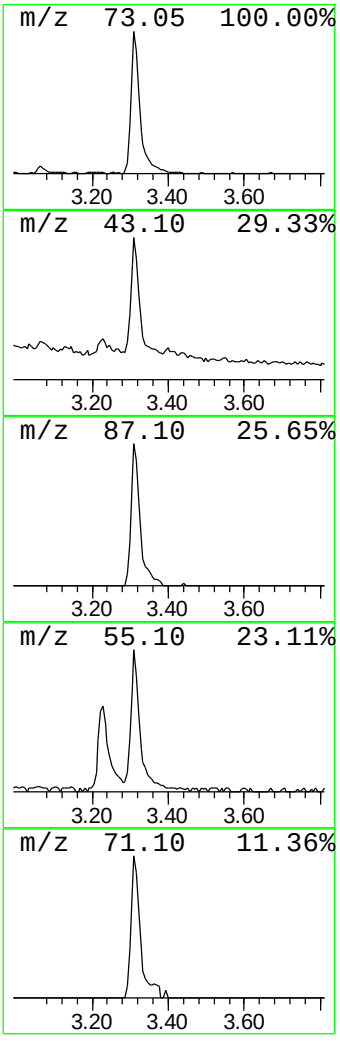
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	3.13 ng	242092	1,4-Dichlorobenzene-d4	8.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

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Acq On : 06 Mar 2018 15:24
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Sample : J1699-45
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : B14

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

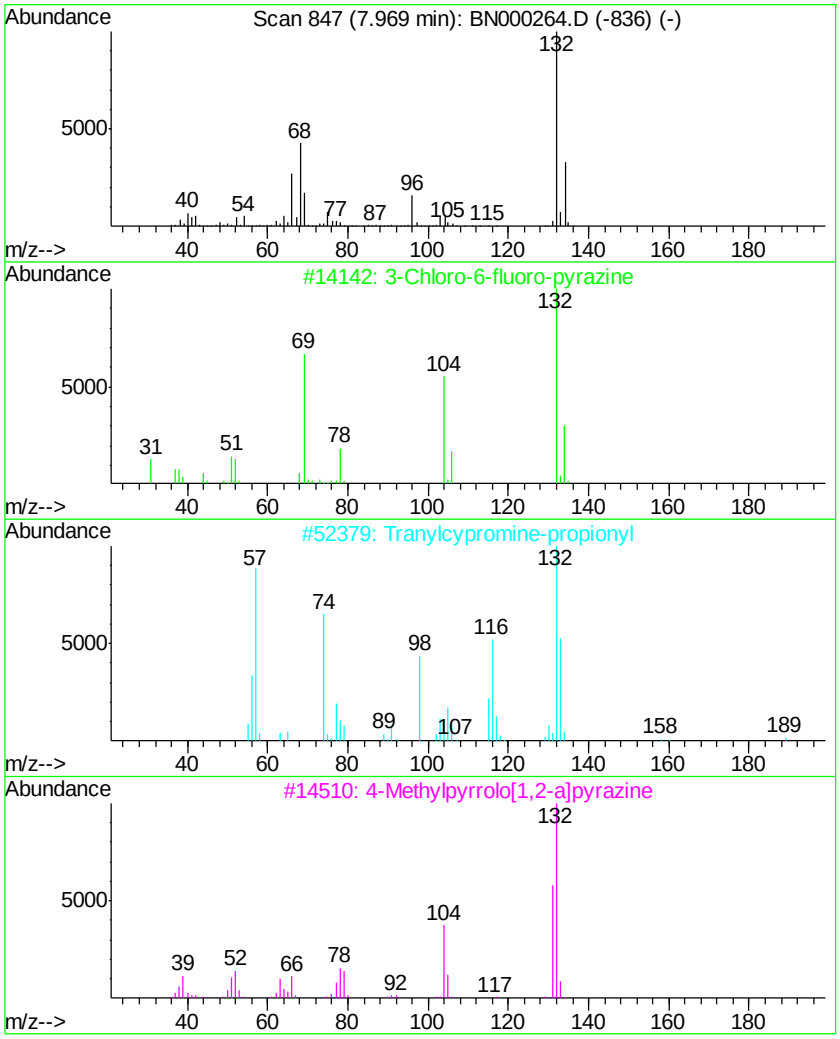
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

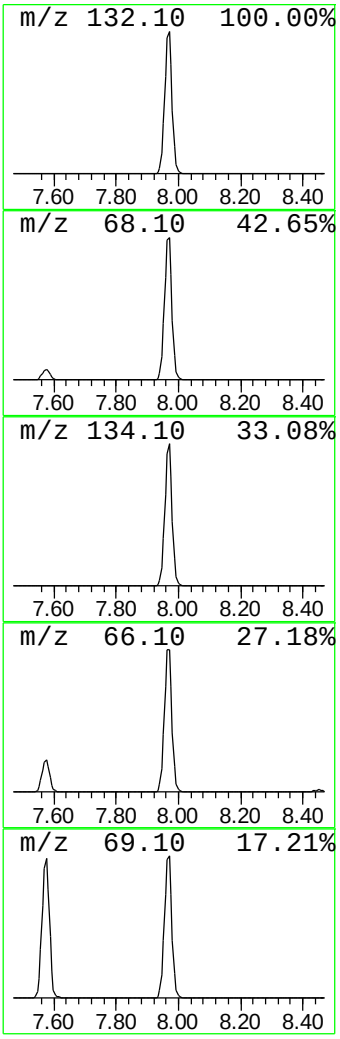
****

Peak Number 3 unknown7.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	63.67 ng	4919540	1,4-Dichlorobenzene-d4	8.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Xenon	132	Xe	007440-63-3	9





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Data File : BN000264.D
Acq On : 06 Mar 2018 15:24
Operator : JU/SJ
Sample : J1699-45
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : B14

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

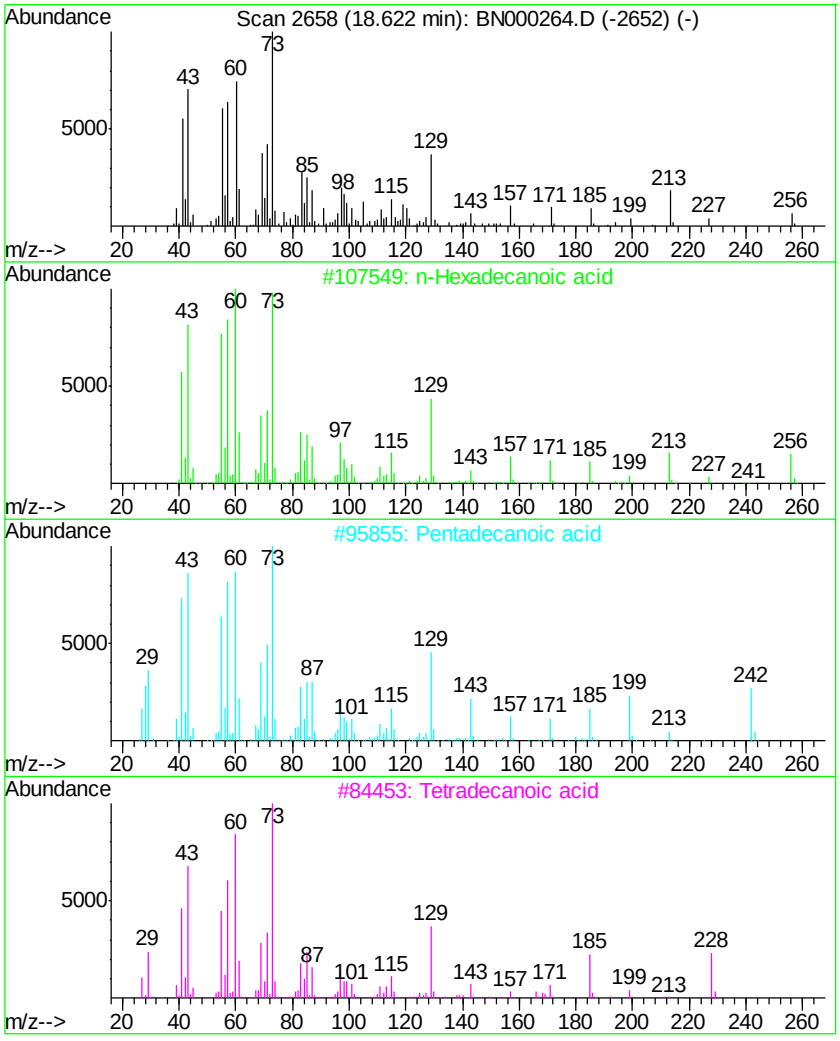
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

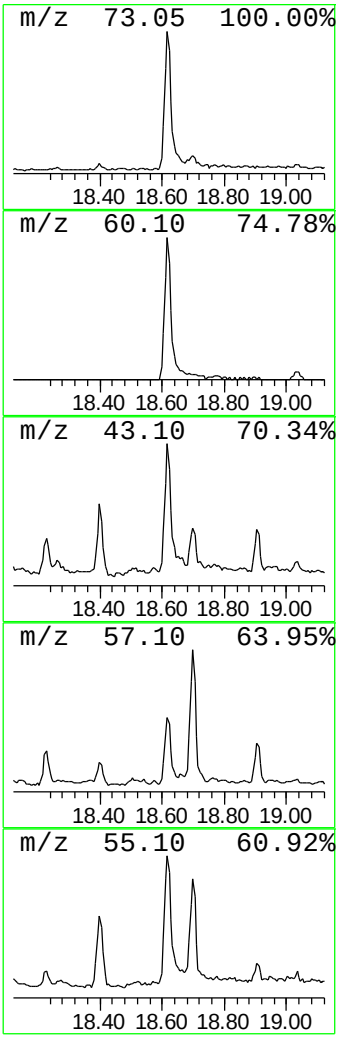
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.62	2.28 ng	438031	Phenanthrene-d10	17.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





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Sample : J1699-45
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : B14

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

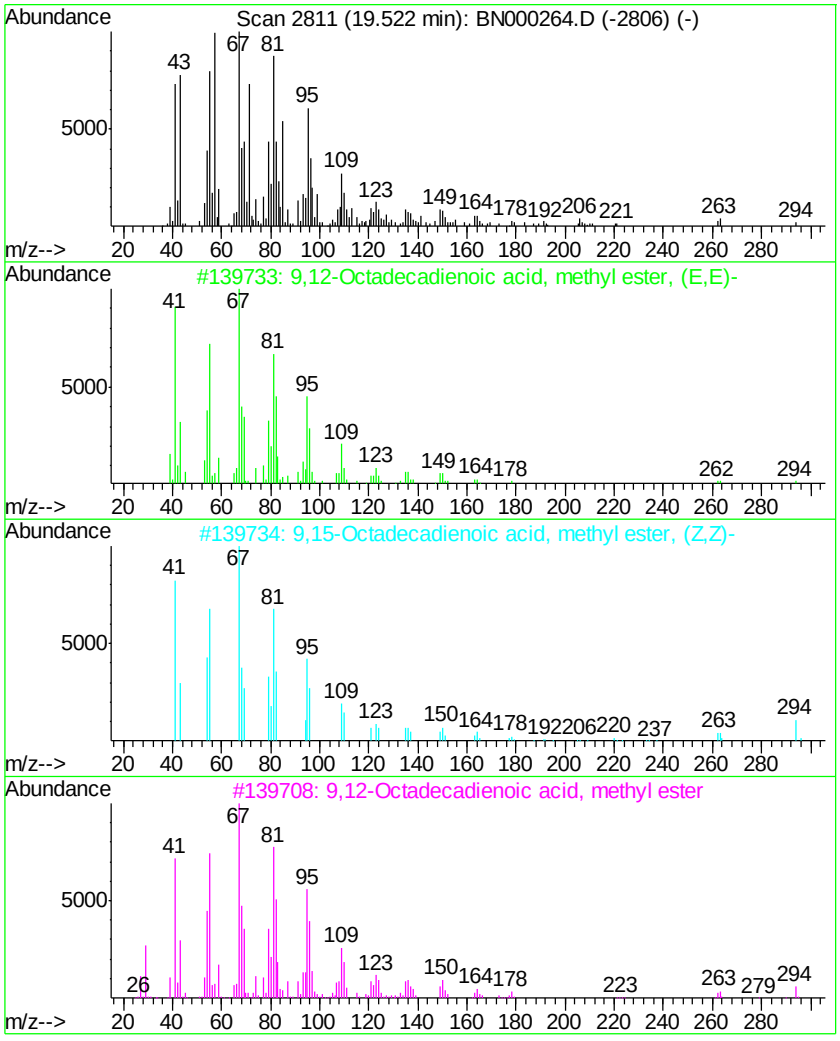
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

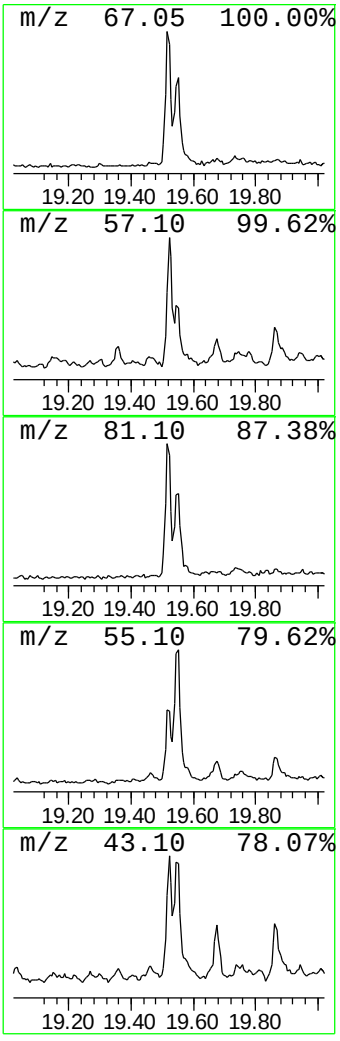
****

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	2.05 ng	394118	Phenanthrene-d10	17.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
5	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	95





Library Search Compound Report

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

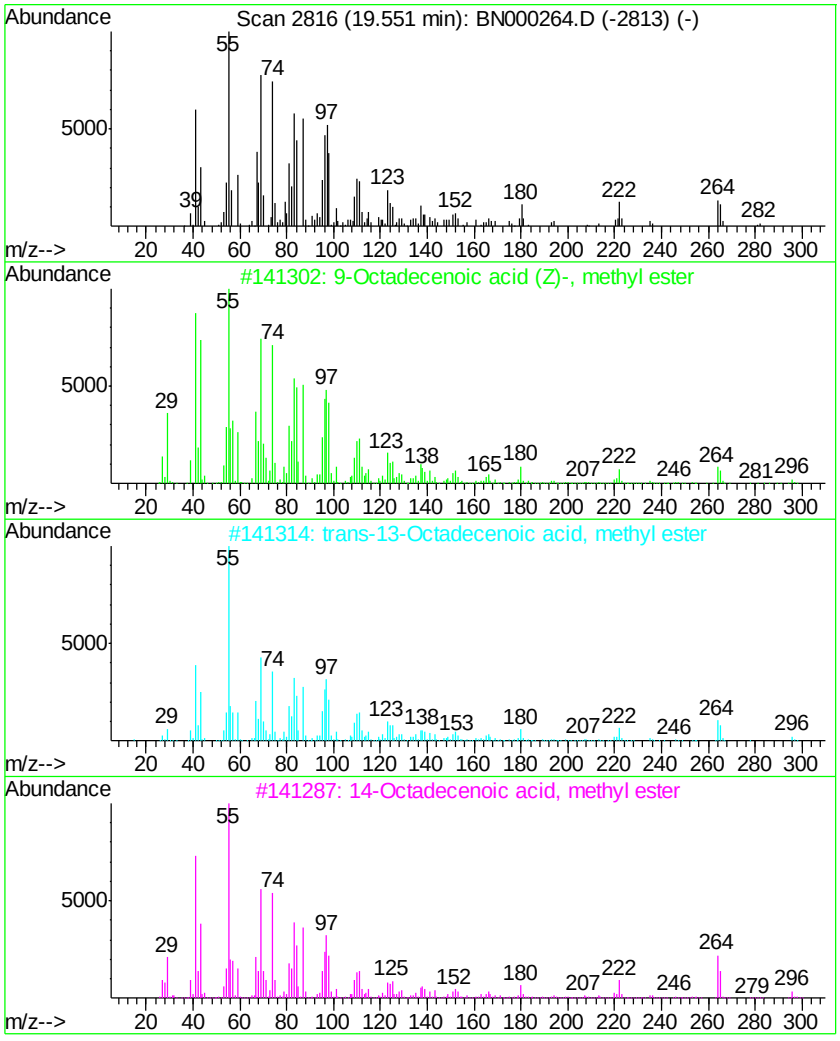
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

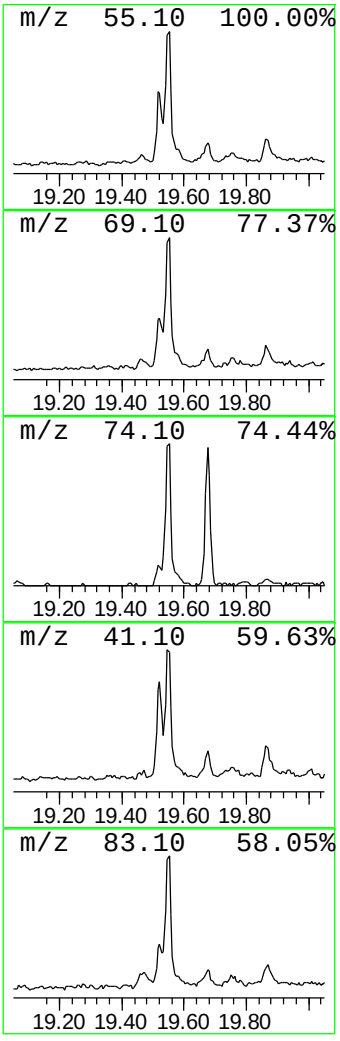
****

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.55	2.89 ng	554189	Phenanthrene-d10	17.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	89
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	76
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	76
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	76





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

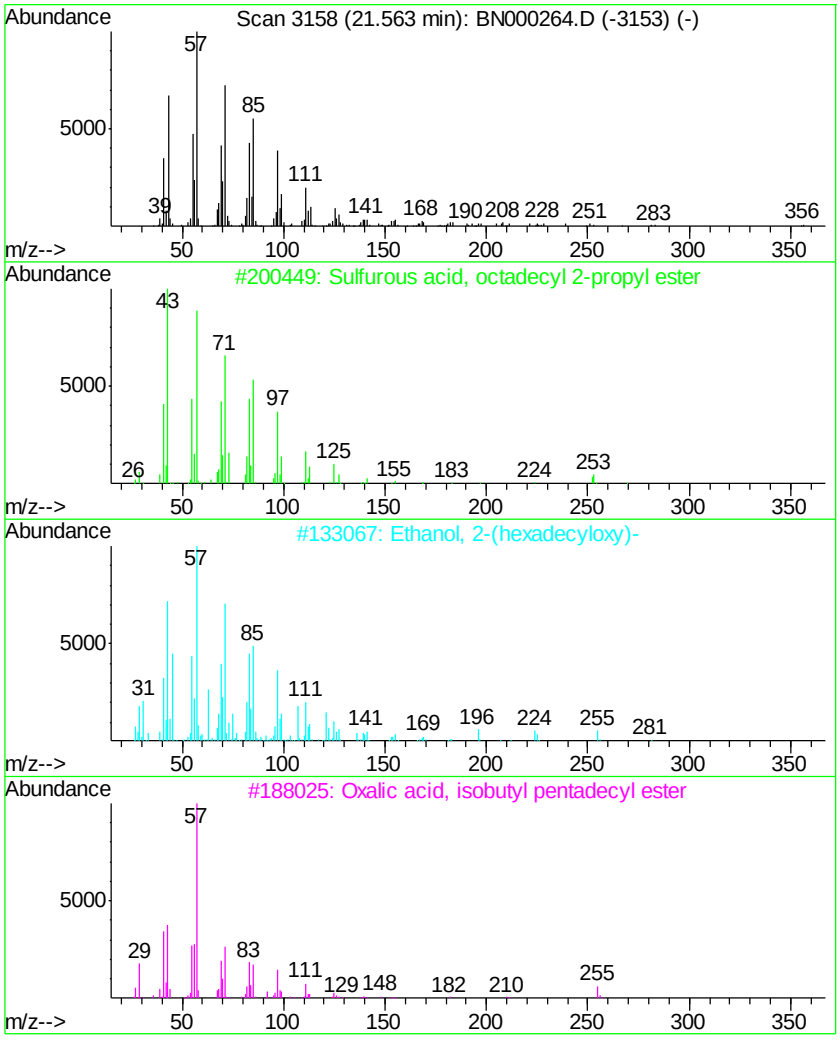
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

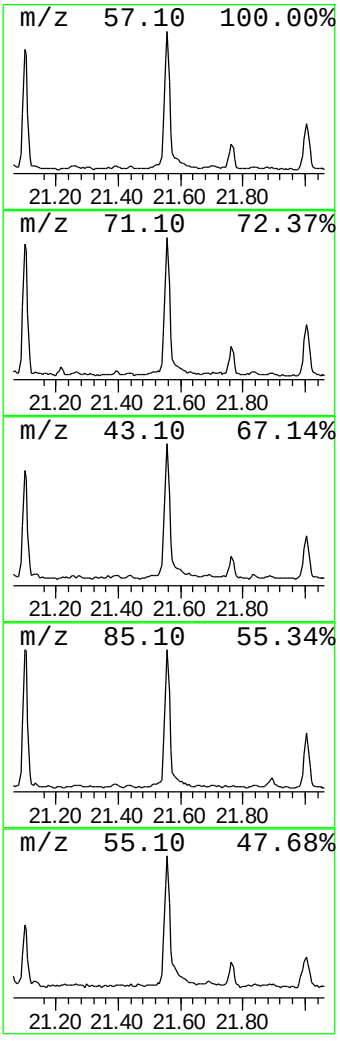
****

Peak Number 8 Sulfurous acid, octadecyl 2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.56	2.66 ng	591514	Chrysene-d12	21.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
2	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
4	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	80
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74





Tentatively Identified Compound (LSC) summary

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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...	3.31	3.1	ng	242092	1	8.45	1545330	20.0
unknown7.97	7.97	63.7	ng	4919540	1	8.45	1545330	20.0
n-Hexadecanoic acid	18.62	2.3	ng	438031	4	17.78	3837840	20.0
9,12-Octadecadien...	19.52	2.0	ng	394118	4	17.78	3837840	20.0
9-Octadecenoic ac...	19.55	2.9	ng	554189	4	17.78	3837840	20.0
Sulfurous acid, o...	21.56	2.7	ng	591514	5	21.89	4443350	20.0