LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020124.D
Acq On : 03 May 2019 22:28
Operator : JU/SJ
Sample : K2635-05 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AU-05-050219-C

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_M\METHODS\8270-BM043019.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	5.363	398	404	414	rVB	492589	706582	16.10%	2.415%
2	6.939	666	672	680	rBV	511179	780851	17.79%	2.668%
3	7.316	729	736	746	rVB	499808	816309	18.60%	2.790%
4	7.787	809	816	823	rBV	644791	979689	22.32%	3.348%
5	8.104	863	870	877	rVB	400274	622030	14.17%	2.126%
6	8.951	1007	1014	1024	rBV	281686	491352	11.19%	1.679%
7	10.580	1284	1291	1297	rVB	791226	1316122	29.98%	4.498%
8	13.045	1704	1710	1716	rVB	768219	1107961	25.24%	3.786%
9	13.233	1732	1742	1749	rBV4	37635	81101	1.85%	0.277%
10	13.886	1848	1853	1858	rVV	96723	146065	3.33%	0.499%
11	14.310	1921	1925	1930	rBV2	83062	104010	2.37%	0.355%
12	14.427	1939	1945	1953	rVB2	1229430	1811302	41.26%	6.190%
13	15.262	2083	2087	2093	rBV2	105245	142157	3.24%	0.486%
14	15.668	2148	2156	2162	rBV3	44351	104487	2.38%	0.357%
15	15.915	2189	2198	2206	rBV	581020	833638	18.99%	2.849%
16	16.127	2229	2234	2242	rBV2	145447	255134	5.81%	0.872%
17	16.921	2364	2369	2372	rBV	147211	174354	3.97%	0.596%
18	16.968	2373	2377	2381	rVB2	64360	89457	2.04%	0.306%
19	17.174	2406	2412	2417	rBV2	1531210	2155982	49.11%	7.368%
20	17.656	2490	2494	2499	rBV	137980	162899	3.71%	0.557%
21	17.833	2520	2524	2530	rVB	541978	644567	14.68%	2.203%
22	18.056	2557	2562	2567	rBV2	121263	179674	4.09%	0.614%
23	18.351	2608	2612	2617	rBV2	110733	139486	3.18%	0.477%
24	18.980	2714	2719	2722	rBV	3682582	4389775	100.00%	15.001%
25	19.015	2722	2725	2737	rVB2	2422040	3094573	70.50%	10.575%
26	19.145	2743	2747	2752	rBV	439531	489603	11.15%	1.673%
27	19.192	2752	2755	2757	rBV3	51691	63401	1.44%	0.217%
28	19.233	2757	2762	2766	rVB	76223	138956	3.17%	0.475%
29	19.333	2776	2779	2789	rVB7	45332	82282	1.87%	0.281%
30	19.562	2815	2818	2821	rBV2	74223	90440	2.06%	0.309%
31	19.592	2821	2823	2829	rVB	60214	91575	2.09%	0.313%
32	19.797	2852	2858	2863	rBV	1317178	1564816	35.65%	5.347%
33	20.103	2907	2910	2913	rVB2	75844	84425	1.92%	0.289%
34	20.245	2931	2934	2937	rBV3	46673	44127	1.01%	0.151%

LSC Area Percent Report

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Operator : JU/SJ
Sample : K2635-05 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AU-05-050219-C

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_M\METHODS\8270-BM043019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.286	2937	2941	2945	rBV6	65781	100926	2.30%	0.345%
36	20.345	2948	2951	2955	rVB4	65062	82475	1.88%	0.282%
37	20.592	2991	2993	2997	rVB3	46195	55716	1.27%	0.190%
38	21.056	3069	3072	3077	rVB4	132300	158558	3.61%	0.542%
39	21.356	3118	3123	3127	rBV	1958736	2418503	55.09%	8.265%
40	23.638	3505	3511	3521	rVB	1268557	2467737	56.22%	8.433%

Sum of corrected areas: 29263097

LSC Report - Integrated Chromatogram

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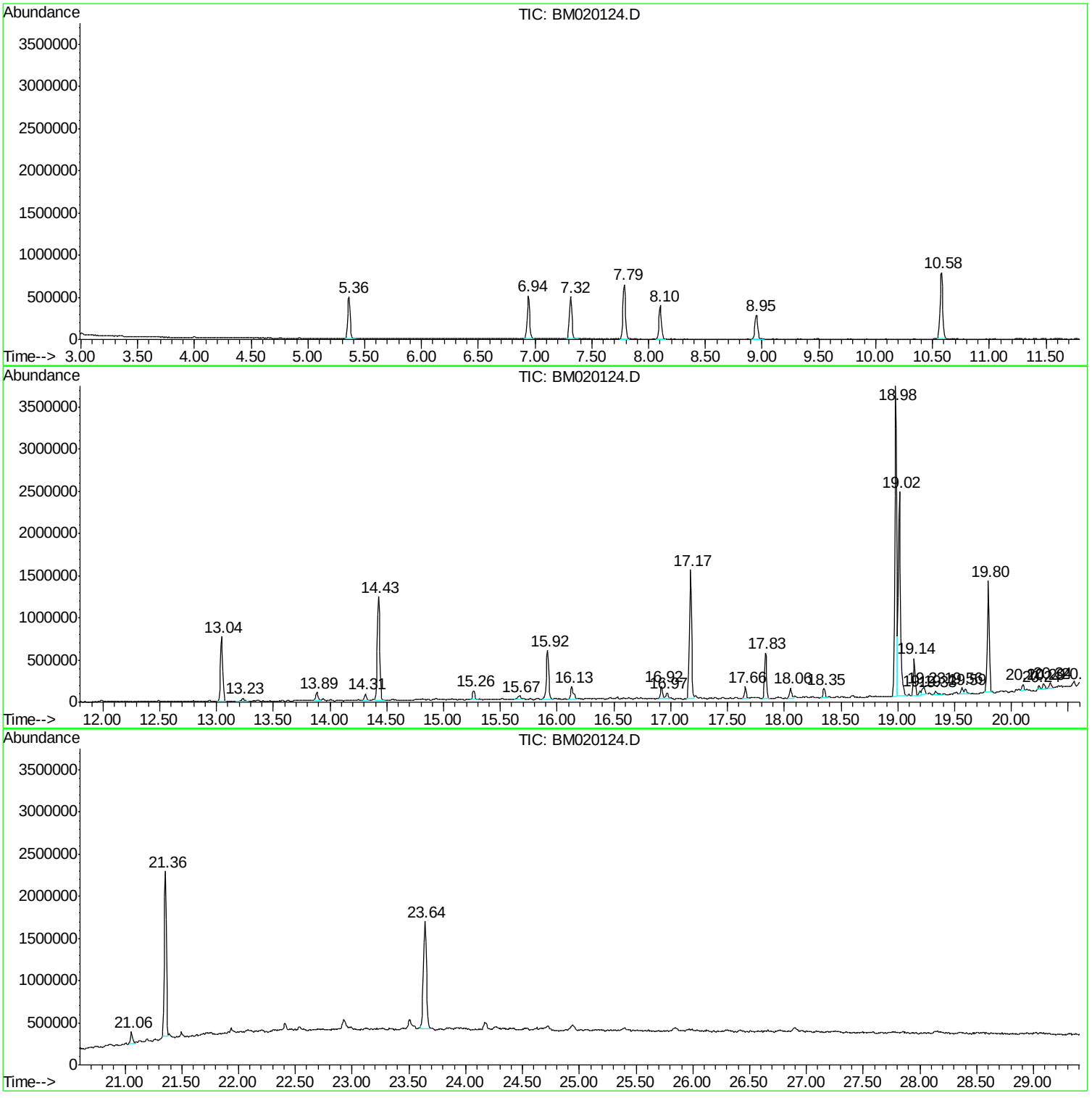
Data File : BM020124.D
Acq On : 03 May 2019 22:28
Operator : JU/SJ
Sample : K2635-05 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AU-05-050219-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Data File : BM020124.D
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Operator : JU/SJ
Sample : K2635-05 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AU-05-050219-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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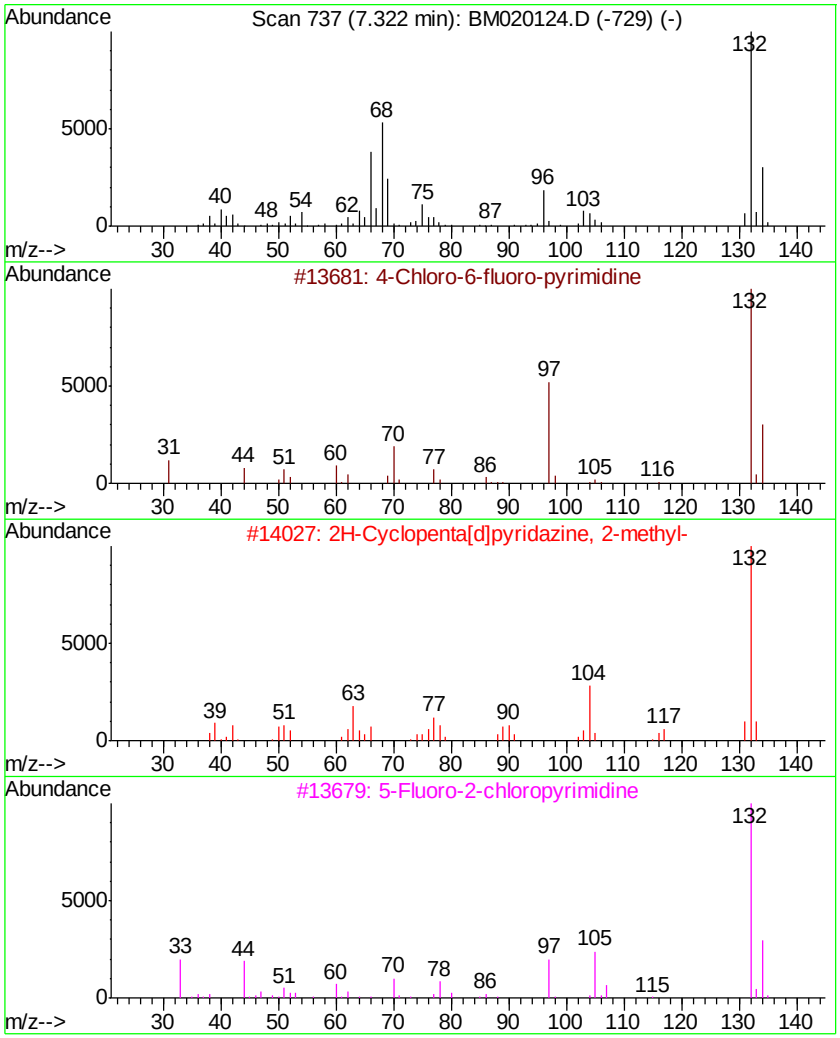
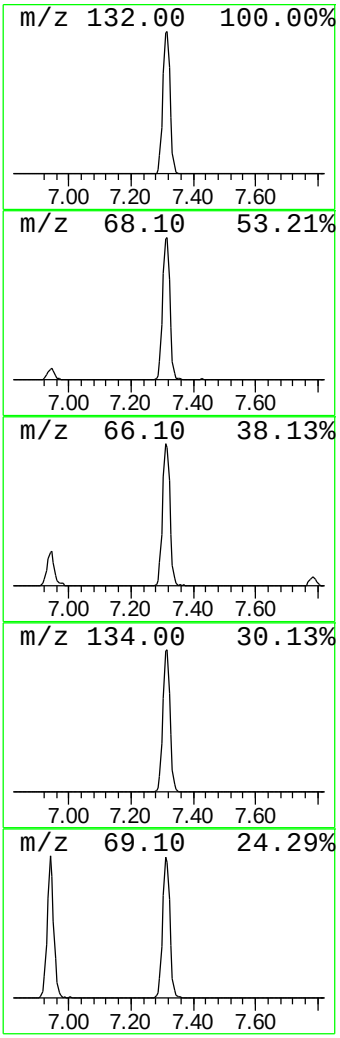
Peak Number 1 unknown7.32 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	16.66 ng	816309	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11





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Data File : BM020124.D
Acq On : 03 May 2019 22:28
Operator : JU/SJ
Sample : K2635-05 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AU-05-050219-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

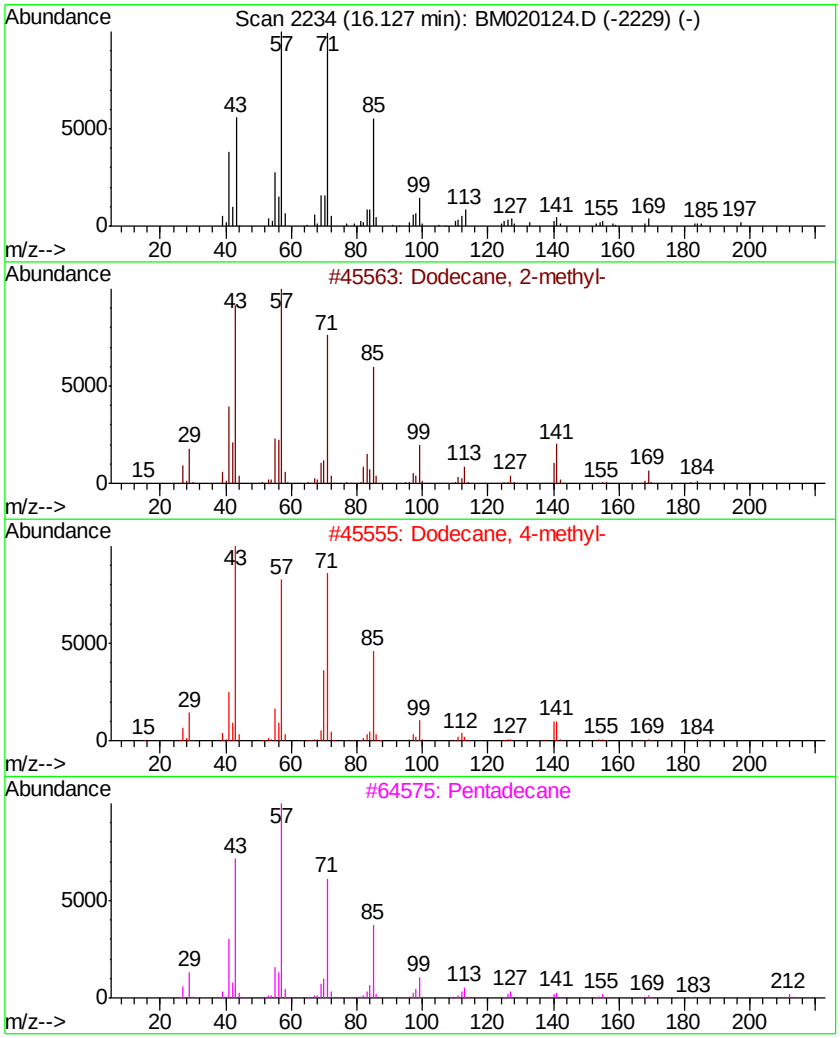
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

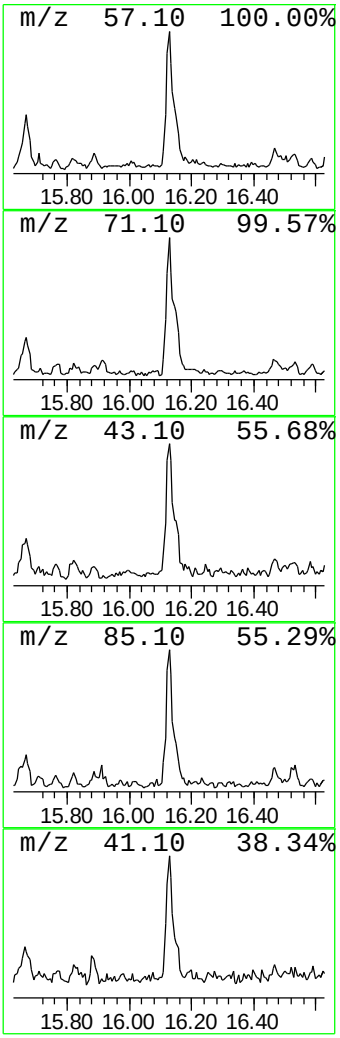
****

Peak Number 3 Dodecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.37 ng	255134	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
2	Dodecane, 4-methyl-	184	C13H28	006117-97-1	87
3	Pentadecane	212	C15H32	000629-62-9	80
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	74
5	Heptacosane	380	C27H56	000593-49-7	72





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Instrument : BNA_M
ClientSampleId : AU-05-050219-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
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TIC Library : C:\DATABASE\NIST02.L
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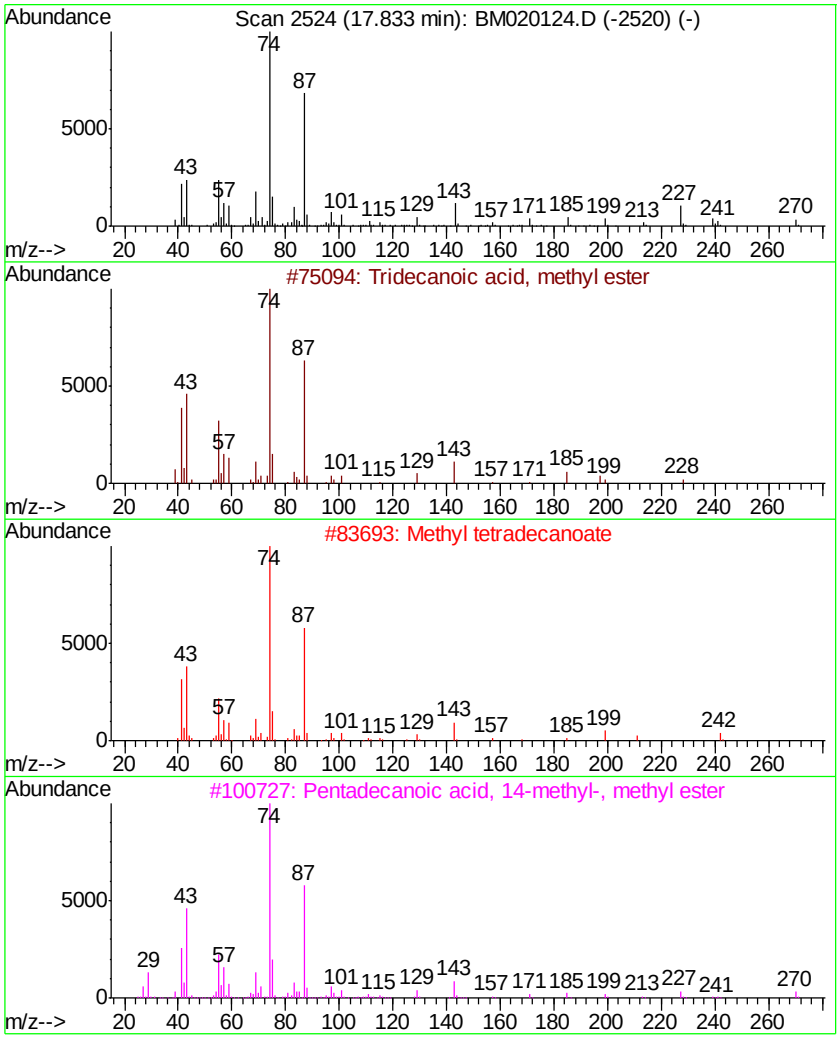
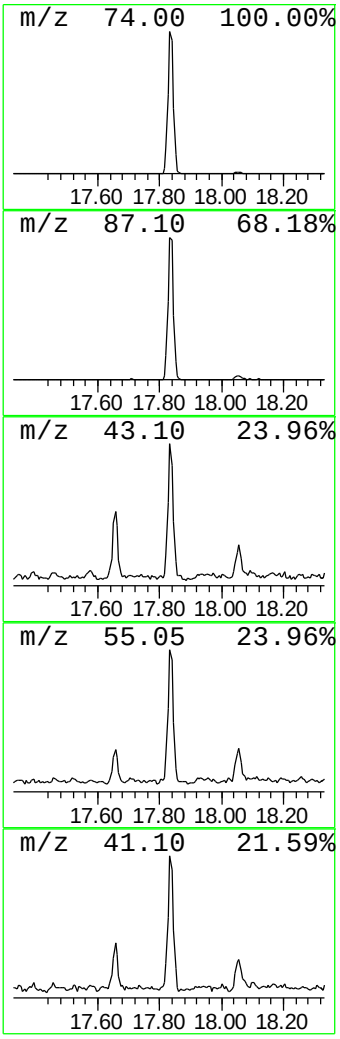
****

Peak Number 4 Tridecanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	5.98 ng	644567	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	92
5	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
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Acq On : 03 May 2019 22:28
Operator : JU/SJ
Sample : K2635-05 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

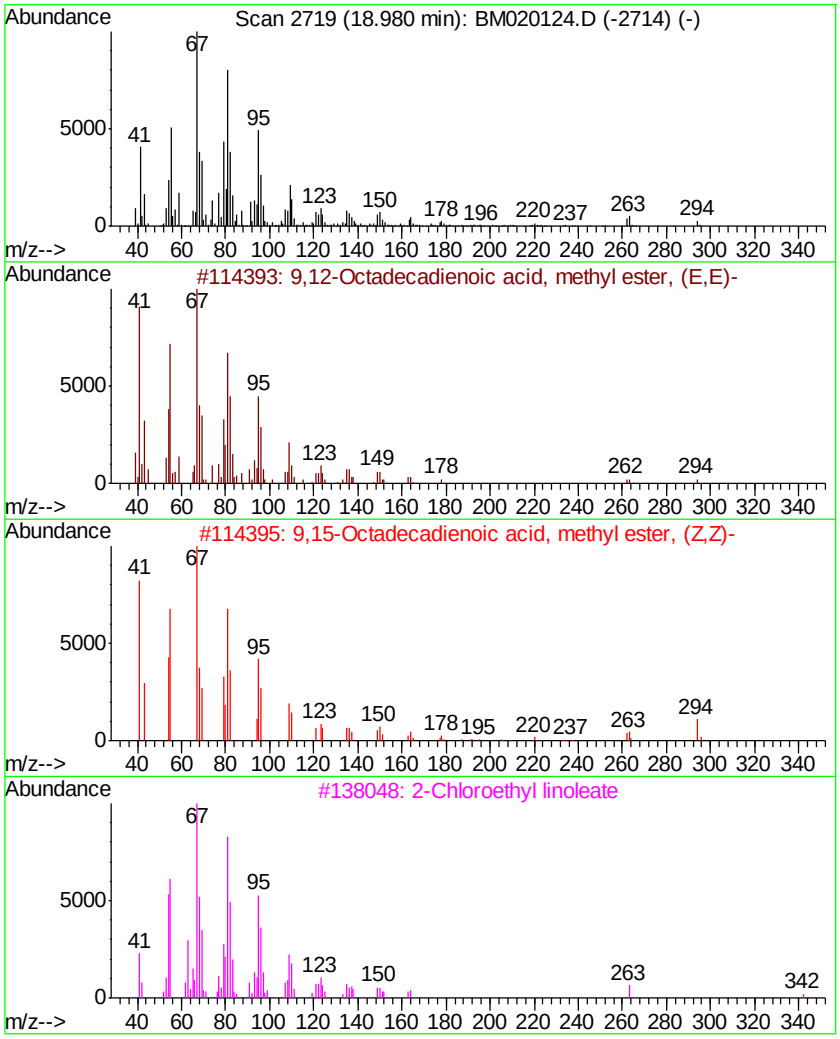
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

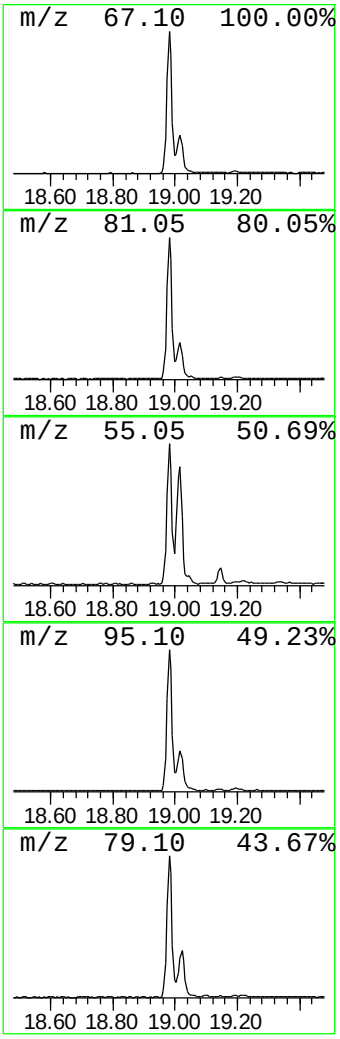
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.98	40.72 ng	4389780	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	96
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
3	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
4	7-Hexadecyne	222	C16H30	074685-28-2	93
5	13-Tetradece-11-yn-1-ol	208	C14H24O	1000131-00-4	93





Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

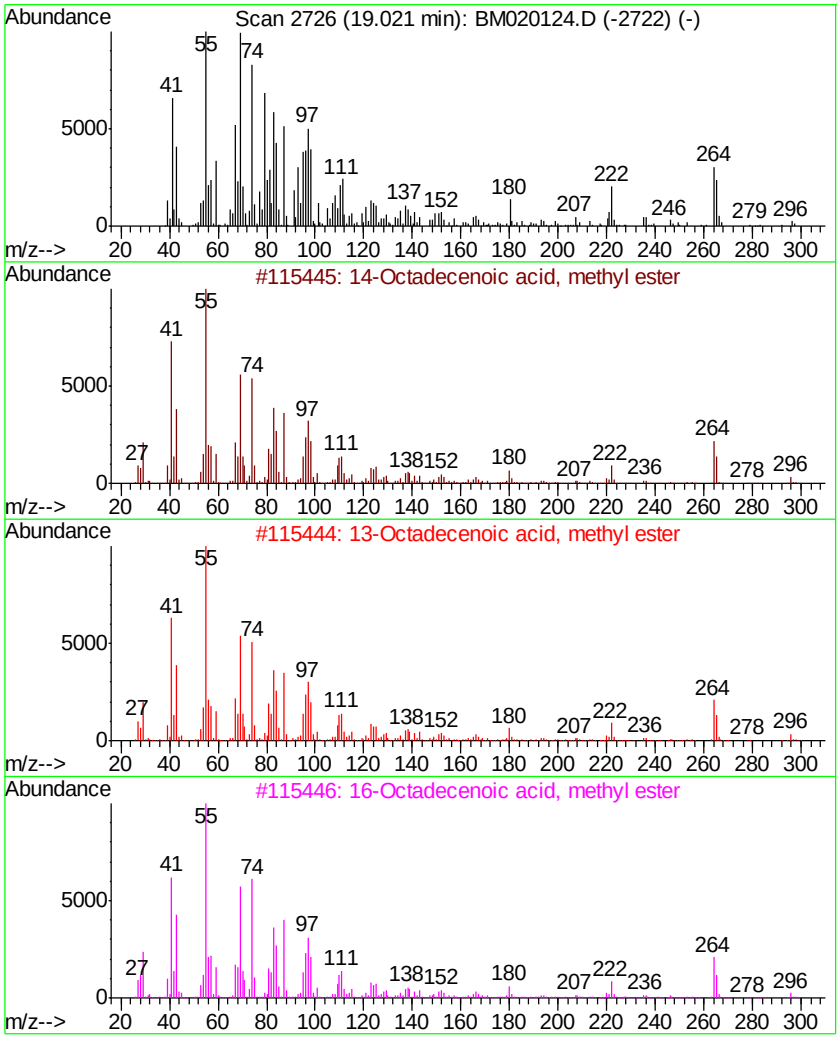
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

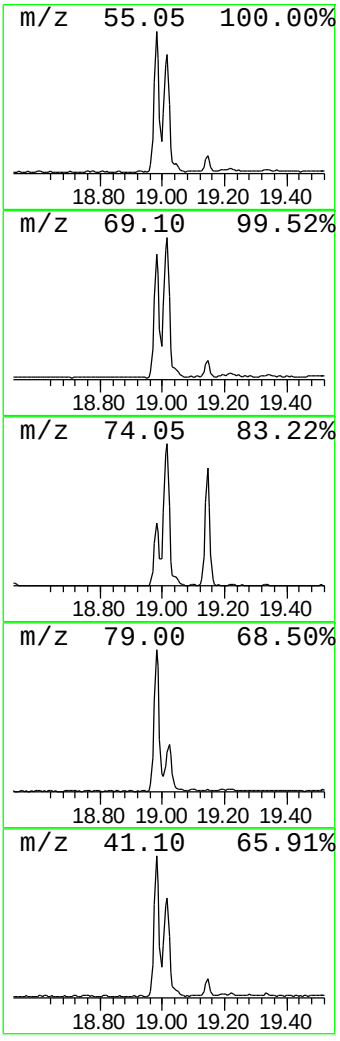
****

Peak Number 6 14-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	28.71 ng	3094570	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

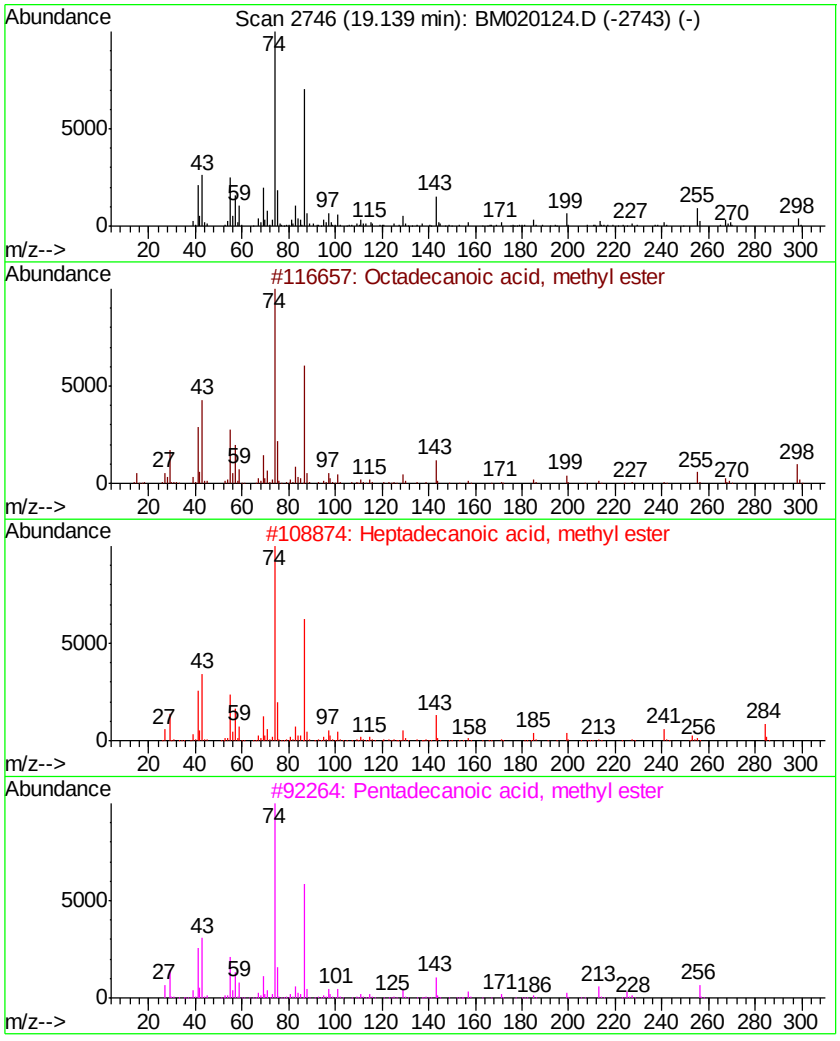
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

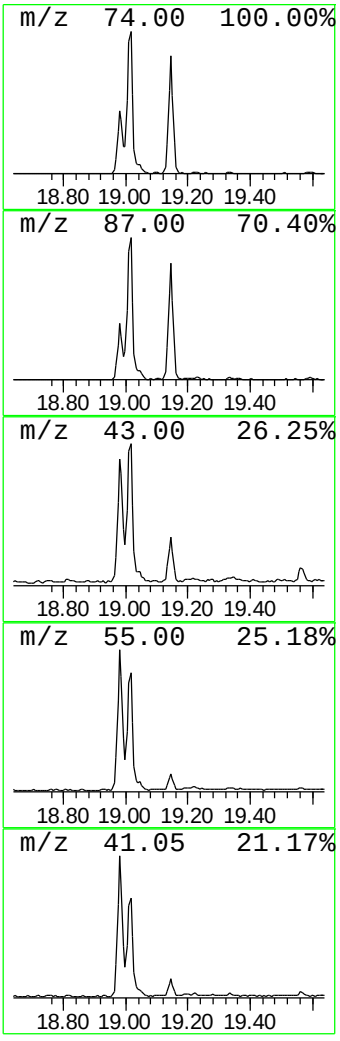
****

Peak Number 7 Octadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	4.54 ng	489603	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	91
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
5	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.32	7.32	16.7	ng	816309	1	7.79	979689	20.0
Dodecane, 2-methyl-	16.13	2.4	ng	255134	4	17.17	2155980	20.0
Tridecanoic acid,...	17.83	6.0	ng	644567	4	17.17	2155980	20.0
9,12-Octadecadien...	18.98	40.7	ng	4389780	4	17.17	2155980	20.0
14-Octadecenoic a...	19.02	28.7	ng	3094570	4	17.17	2155980	20.0
Octadecanoic acid...	19.14	4.5	ng	489603	4	17.17	2155980	20.0