LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.534	56	59	70	rBV	25535	39035	4.45%	0.534%
2	5.475	383	389	402	rVB	363123	514725	58.63%	7.043%
3	7.110	661	667	678	rVB	353410	544335	62.00%	7.448%
4	7.587	743	748	756	rVB3	5007	9649	1.10%	0.132%
5	7.928	800	806	814	rVB	101880	156507	17.83%	2.142%
6	9.104	999	1006	1015	rBV	219338	346395	39.46%	4.740%
7	10.739	1278	1284	1290	rBV	132735	216221	24.63%	2.959%
8	10.798	1290	1294	1302	rVB	26465	39245	4.47%	0.537%
9	11.386	1388	1394	1401	rBV	6843	10175	1.16%	0.139%
10	12.475	1574	1579	1584	rVB	6514	9107	1.04%	0.125%
11	13.204	1696	1703	1709	rBV	505142	716318	81.59%	9.802%
12	13.392	1728	1735	1743	rVB2	7731	11679	1.33%	0.160%
13	14.033	1839	1844	1851	rVB	20358	30341	3.46%	0.415%
14	14.427	1904	1911	1915	rBV3	4089	10165	1.16%	0.139%
15	14.469	1915	1918	1924	rVB3	10073	13438	1.53%	0.184%
16	14.580	1931	1937	1943	rVB	187612	279936	31.89%	3.831%
17	15.416	2073	2079	2083	rVB2	11238	15067	1.72%	0.206%
18	15.821	2140	2148	2154	rBV2	6852	13039	1.49%	0.178%
19	16.068	2180	2190	2195	rBV	397996	553620	63.06%	7.575%
20	16.274	2220	2225	2226	rBV	12439	13372	1.52%	0.183%
21	16.298	2226	2229	2233	rVB2	17418	23839	2.72%	0.326%
22	16.968	2338	2343	2349	rBV	148043	200927	22.89%	2.749%
23	17.063	2353	2359	2363	rVB	9813	13487	1.54%	0.185%
24	17.110	2363	2367	2371	rBV2	8592	13642	1.55%	0.187%
25	17.315	2396	2402	2406	rBV	223595	307776	35.06%	4.211%
26	17.357	2406	2409	2417	rVB	60532	79439	9.05%	1.087%
27	17.445	2420	2424	2428	rBV	14286	17560	2.00%	0.240%
28	17.715	2467	2470	2479	rVB2	7317	11558	1.32%	0.158%
29	17.792	2479	2483	2487	rBV	9045	11876	1.35%	0.163%
30	18.198	2546	2552	2556	rBV2	103345	150009	17.09%	2.053%
31	18.380	2577	2583	2587	rVV2	11277	23470	2.67%	0.321%
32	18.486	2597	2601	2605	rBV3	9538	11300	1.29%	0.155%
33	18.680	2630	2634	2638	rBV2	6870	8798	1.00%	0.120%
34	18.727	2638	2642	2646	rVV2	7945	10621	1.21%	0.145%
35	19.109	2701	2707	2711	rBV3	8660	17599	2.00%	0.241%
36	19.356	2744	2749	2755	rVB	126635	168914	19.24%	2.311%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.462	2763	2767	2773	rBV2	42910	62292	7.10%	0.852%
38	19.686	2801	2805	2807	rBV3	21966	28578	3.26%	0.391%
39	19.721	2807	2811	2819	rVB	97490	140242	15.97%	1.919%
40	19.786	2819	2822	2827	rBV4	7249	10719	1.22%	0.147%
41	19.915	2838	2844	2849	rVV	686781	877936	100.00%	12.013%
42	19.962	2849	2852	2856	rVB	7061	9181	1.05%	0.126%
43	20.068	2861	2870	2875	rBV4	28130	48557	5.53%	0.664%
44	20.221	2891	2896	2900	rVB3	25644	45347	5.17%	0.621%
45	20.309	2908	2911	2914	rBV	10694	12543	1.43%	0.172%
46	20.368	2914	2921	2926	rBV5	17997	37992	4.33%	0.520%
47	20.456	2931	2936	2941	rVV	60819	78326	8.92%	1.072%
48	20.545	2948	2951	2956	rVB2	16648	19442	2.21%	0.266%
49	20.645	2965	2968	2972	rBV3	13120	18793	2.14%	0.257%
50	20.709	2976	2979	2982	rVV4	16098	20329	2.32%	0.278%
51	20.745	2982	2985	2990	rVB7	7437	10194	1.16%	0.139%
52	20.945	3017	3019	3022	rBV	8894	9405	1.07%	0.129%
53	21.027	3029	3033	3040	rBV3	41748	57979	6.60%	0.793%
54	21.162	3050	3056	3065	rVB5	125357	190758	21.73%	2.610%
55	21.368	3087	3091	3093	rBV3	40225	53631	6.11%	0.734%
56	21.456	3100	3106	3110	rBV2	294112	427785	48.73%	5.854%
57	21.492	3110	3112	3117	rVB	53402	64700	7.37%	0.885%
58	23.039	3371	3375	3380	rBV	35383	70454	8.02%	0.964%
59	23.615	3470	3473	3481	rVB	40651	72659	8.28%	0.994%
60	23.715	3484	3490	3496	rBV2	177845	327014	37.25%	4.475%

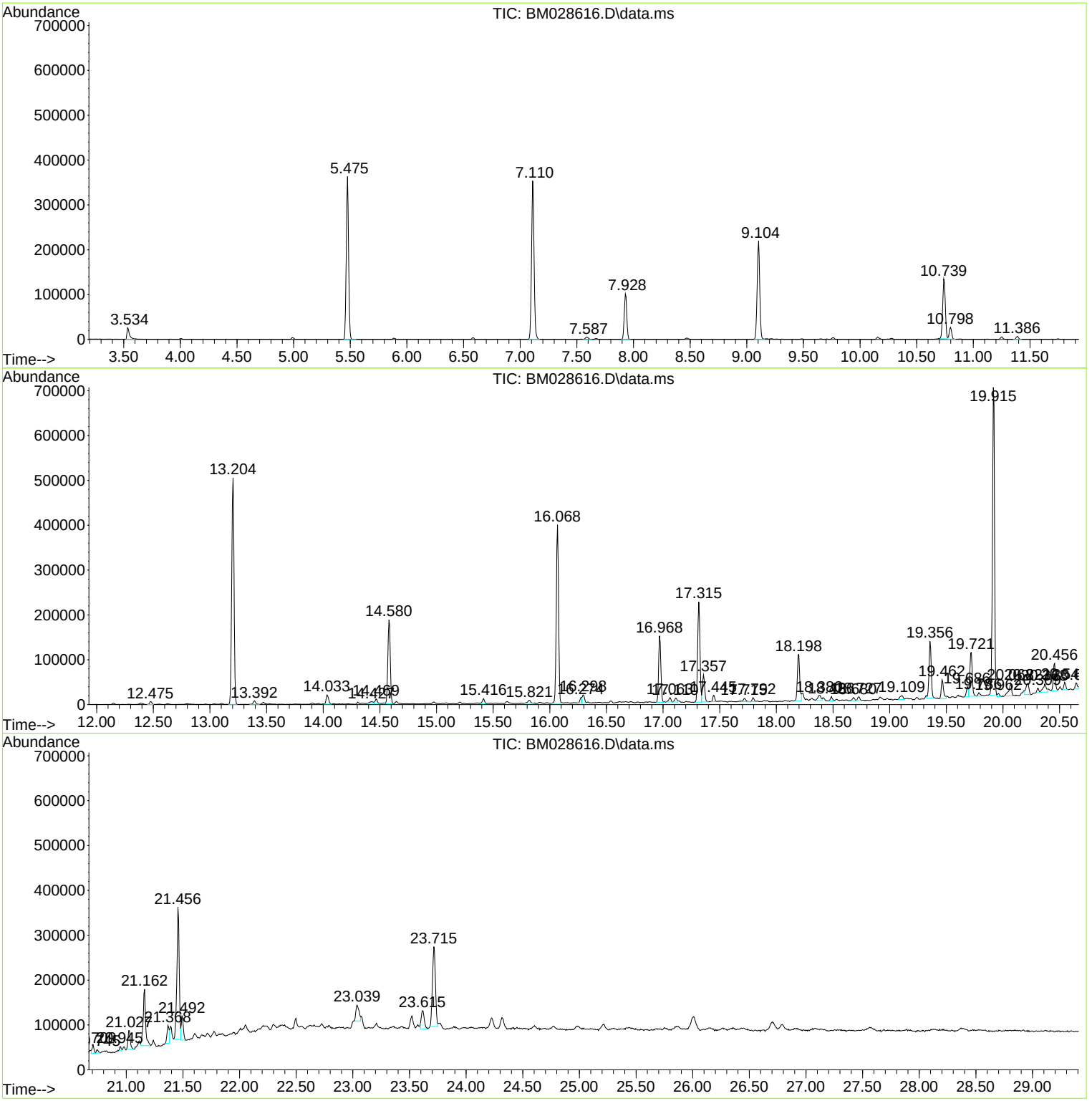
Sum of corrected areas: 7308040

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

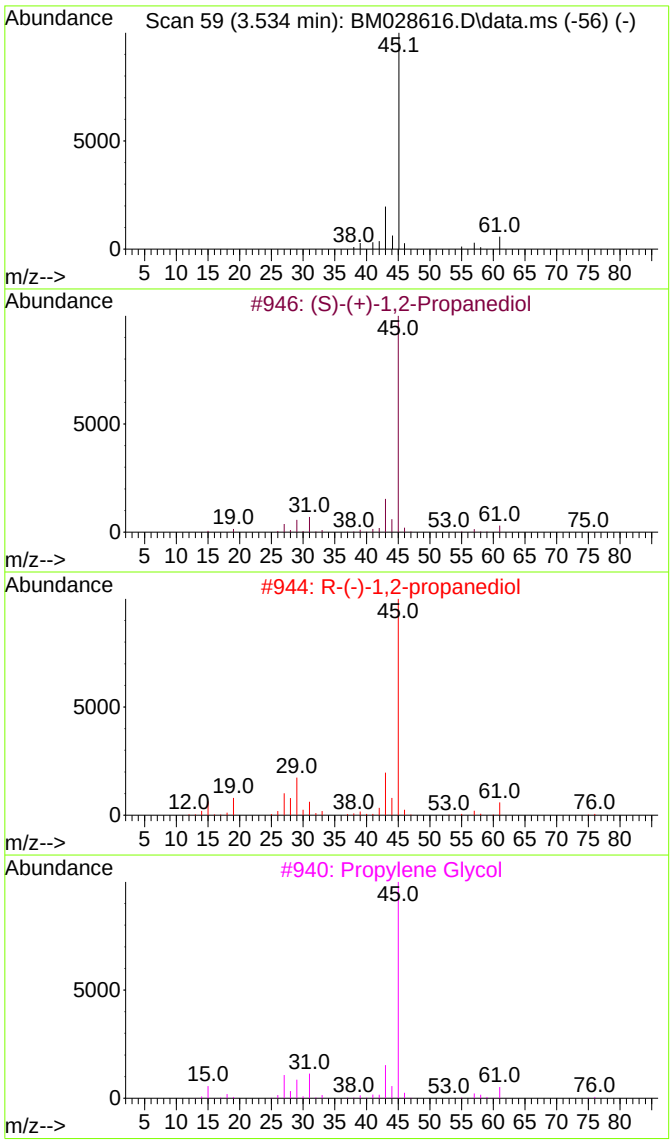
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

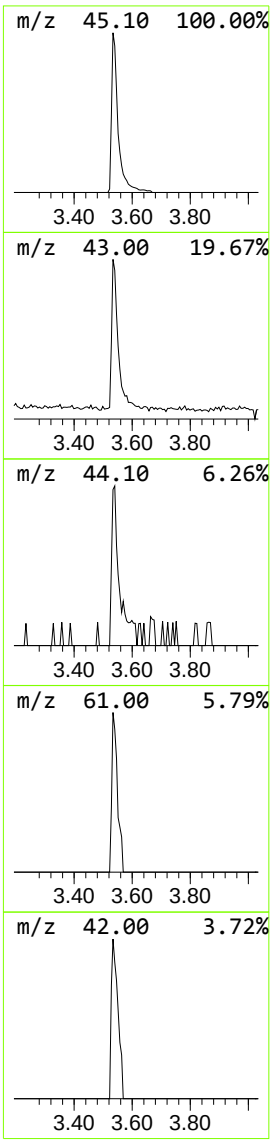
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.534	4.99 ng	39035	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

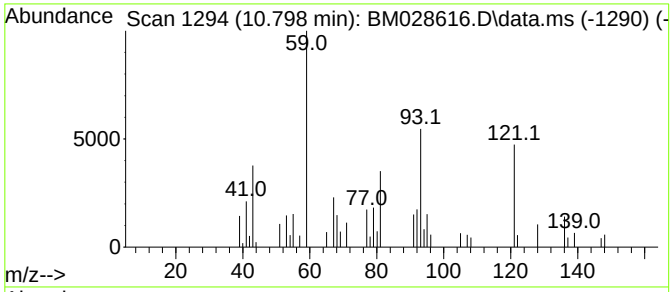
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

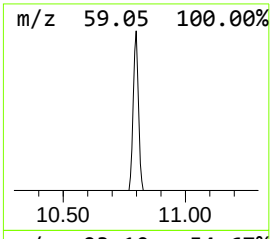
****

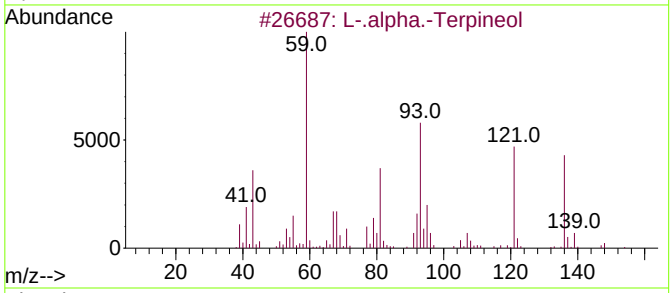
Peak Number 2 L-.alpha.-Terpineol Concentration Rank 5

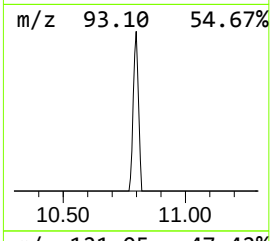
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	3.63 ng	39245	Naphthalene-d8	10.739

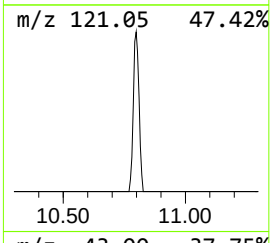
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-.alpha.-Terpineol	154	C10H18O	010482-56-1	64
2	Camphene	136	C10H16	000079-92-5	46
3	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	41
4	Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	001461-27-4	38
5	3-Carene	136	C10H16	013466-78-9	38

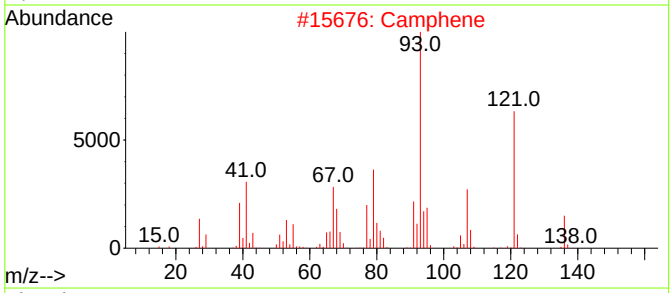


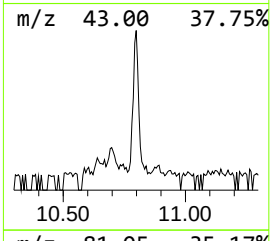


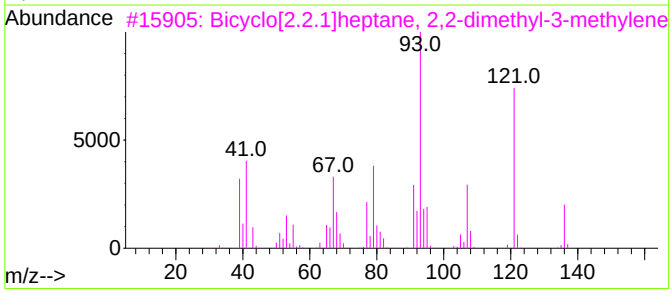


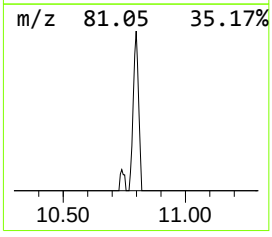












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

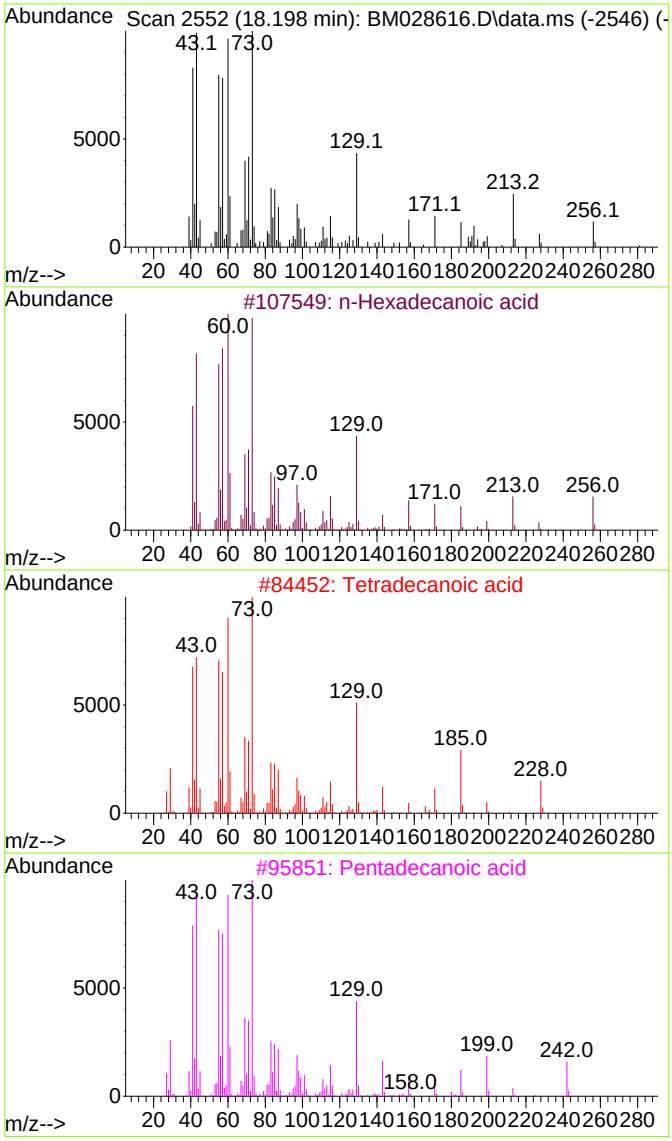
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

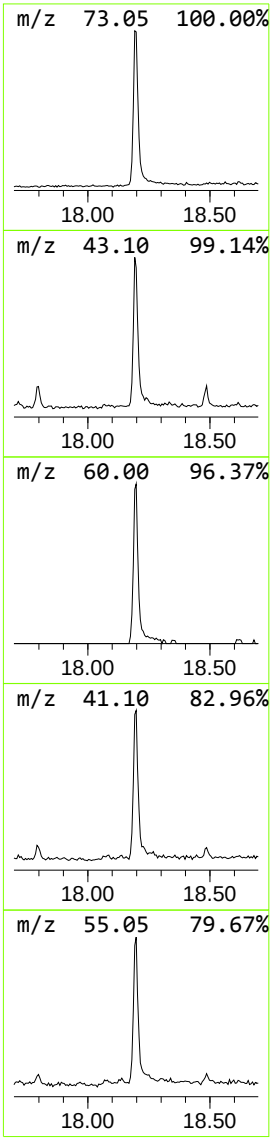
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	9.75 ng	150009	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

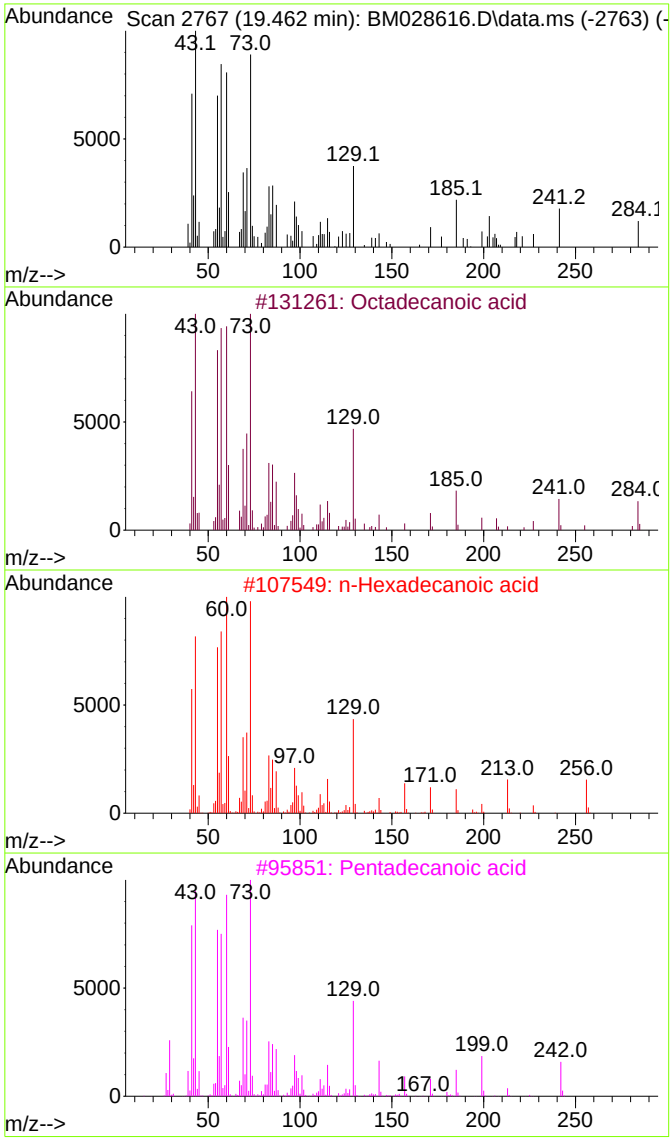
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

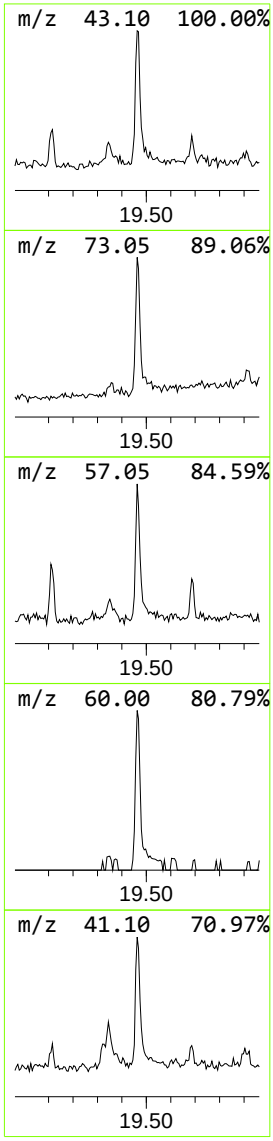
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	2.91 ng	62292	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

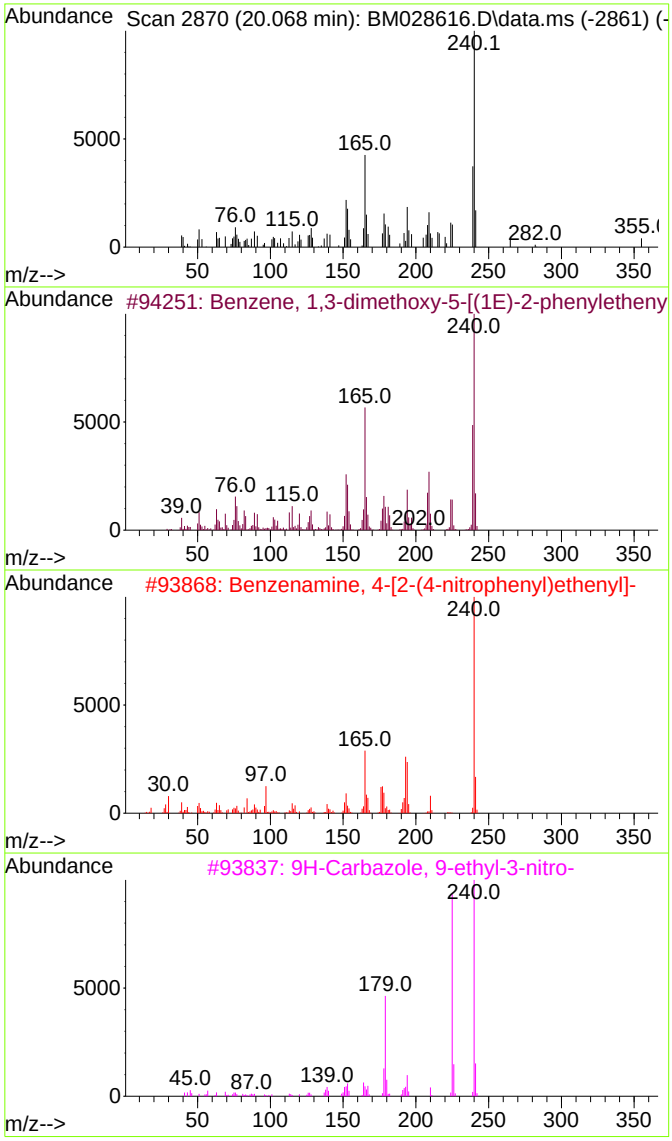
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

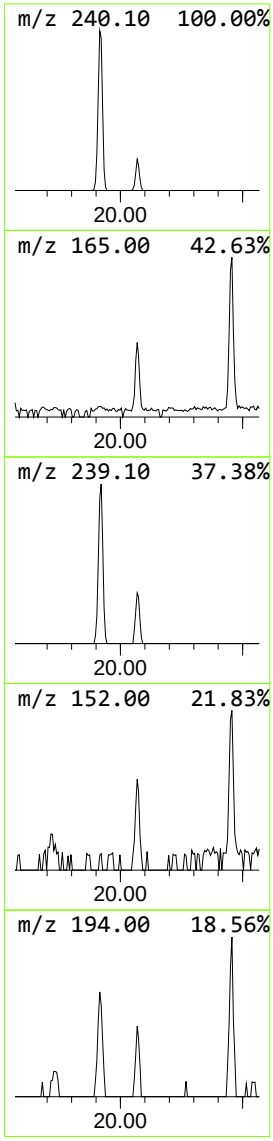
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,3-dimethoxy-5-[(... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.068	2.27 ng	48557	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethoxy-5-[(1E)-2...	240	C16H16O2	021956-56-9	97
2	Benzenamine, 4-[2-(4-nitrophenyl...	240	C14H12N2O2	004629-58-7	60
3	9H-Carbazole, 9-ethyl-3-nitro-	240	C14H12N2O2	000086-20-4	50
4	Naphtho[2,1-b:3,4-b']difuran, 2,...	240	C16H16O2	068873-19-8	49
5	[1,1'-Biphenyl]-4,4'-diamine, 3,...	240	C16H20N2	054827-17-7	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.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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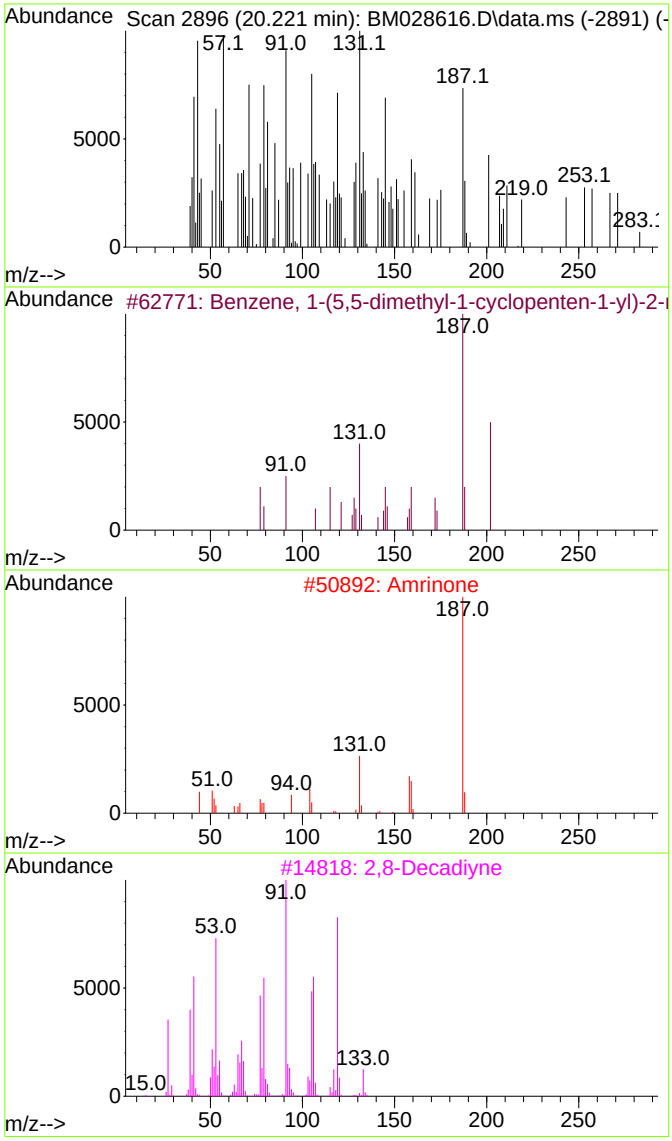
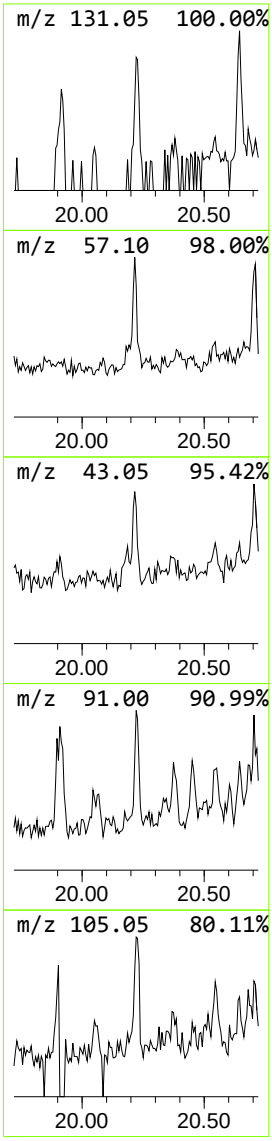
Peak Number 6 unknown20.221 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.221	2.12 ng	45347	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(5,5-dimethyl-1-cyclo...	202	C14H18O	039877-93-5	38
2	Amrinone	187	C10H9N3O	060719-84-8	22
3	2,8-Decadiyne	134	C10H14	004116-93-2	22
4	Bicyclo[4.1.0]heptane,-3-cyclopr...	208	C13H20O2	1000222-97-2	18
5	5,9-Tetradecadiyne	190	C14H22	051255-61-9	16





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Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-RBR-200035

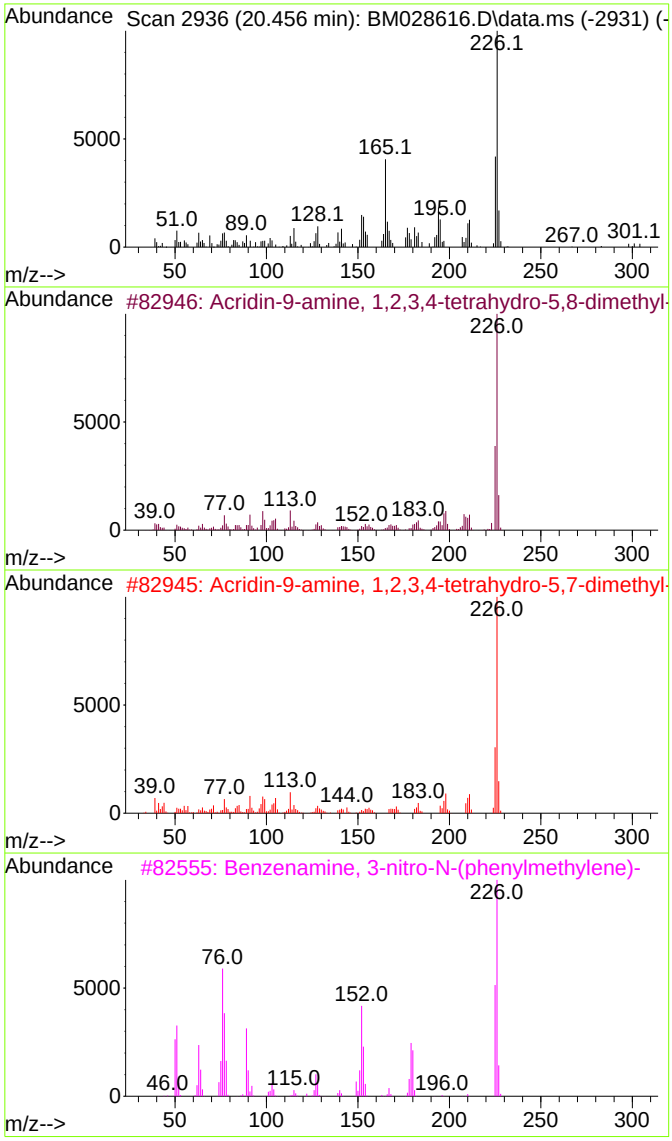
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

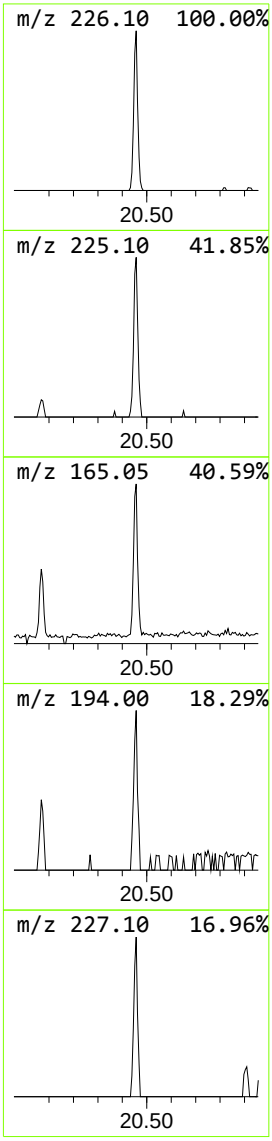
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.456	3.66 ng	78326	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	62
2	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	58
3	Benzenamine, 3-nitro-N-(phenylme...	226	C13H10N2O2	005341-44-6	55
4	N,N-Dimethylindoaniline	226	C14H14N2O	002150-58-5	53
5	Benzenamine, N-[(4-nitrophenyl)m...	226	C13H10N2O2	000785-80-8	46





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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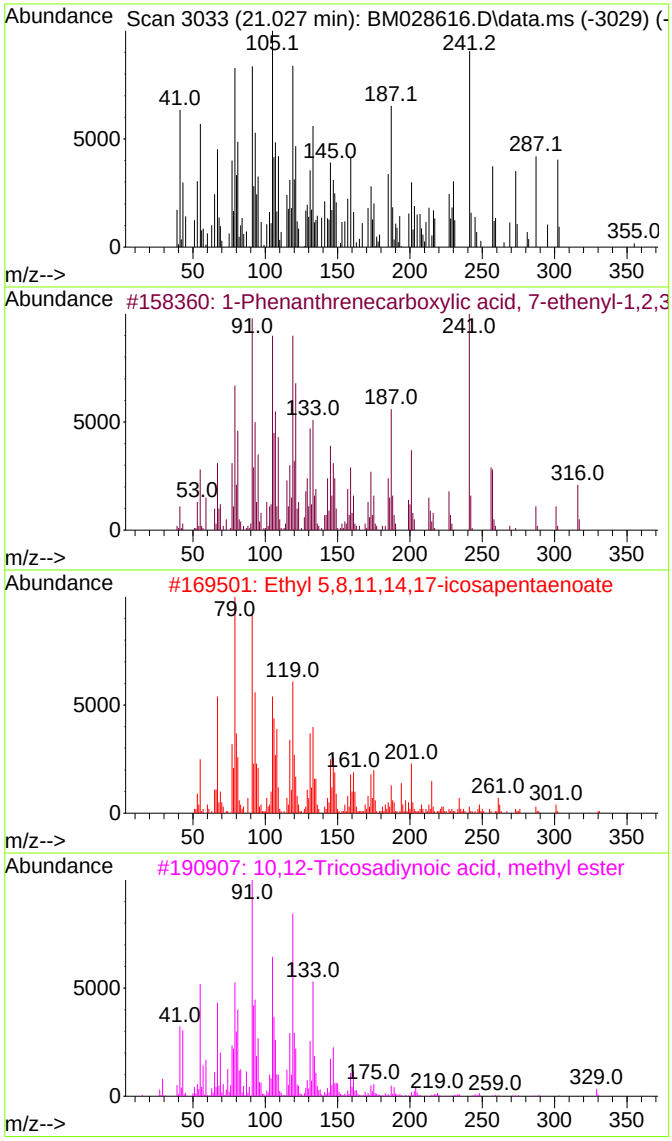
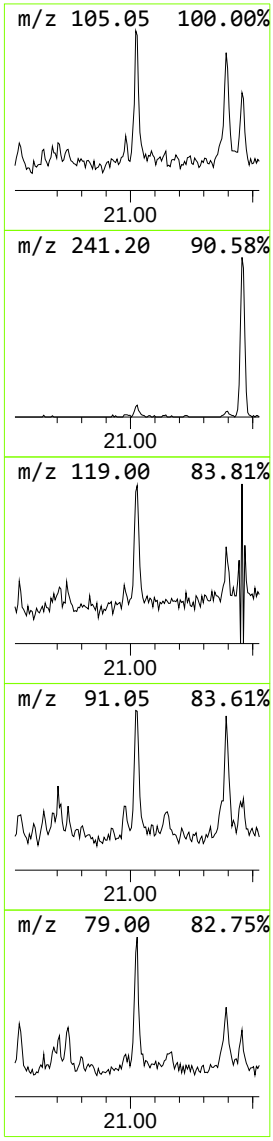
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Phenanthrenecarboxylic ac... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	2.71 ng	57979	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenanthrenecarboxylic acid, 7...	316	C21H32O2	001686-62-0	70
2	Ethyl 5,8,11,14,17-icosapentaenoate	330	C22H34O2	084494-70-2	20
3	10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1000333-59-4	18
4	Methyl 10,12-pentacosadiynoate	388	C26H44O2	1000342-58-7	18
5	2-Cyano-N-(4-(2,6-dimethyl-4-mor...	273	C15H19N3O2	1000332-12-1	18





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Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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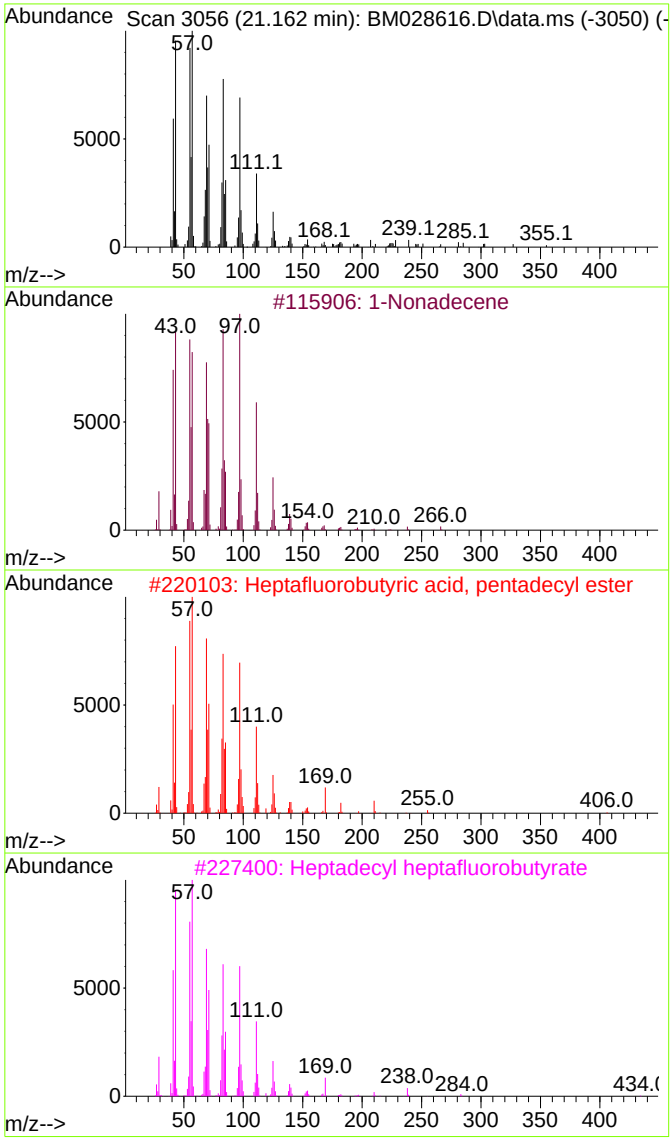
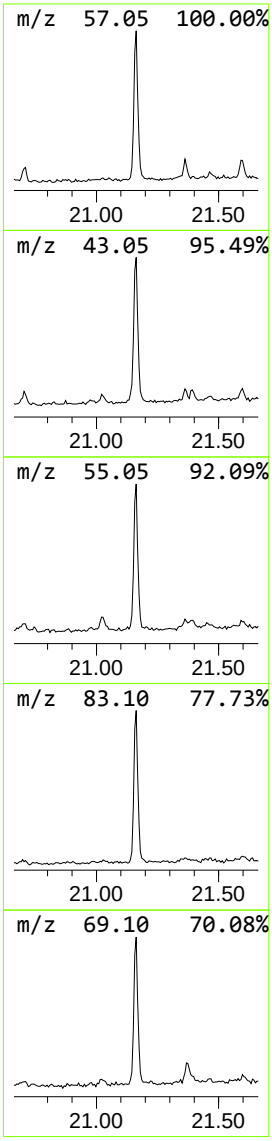
****

Peak Number 9 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	8.92 ng	190758	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





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Instrument :
BNA_M
ClientSampleId :
RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
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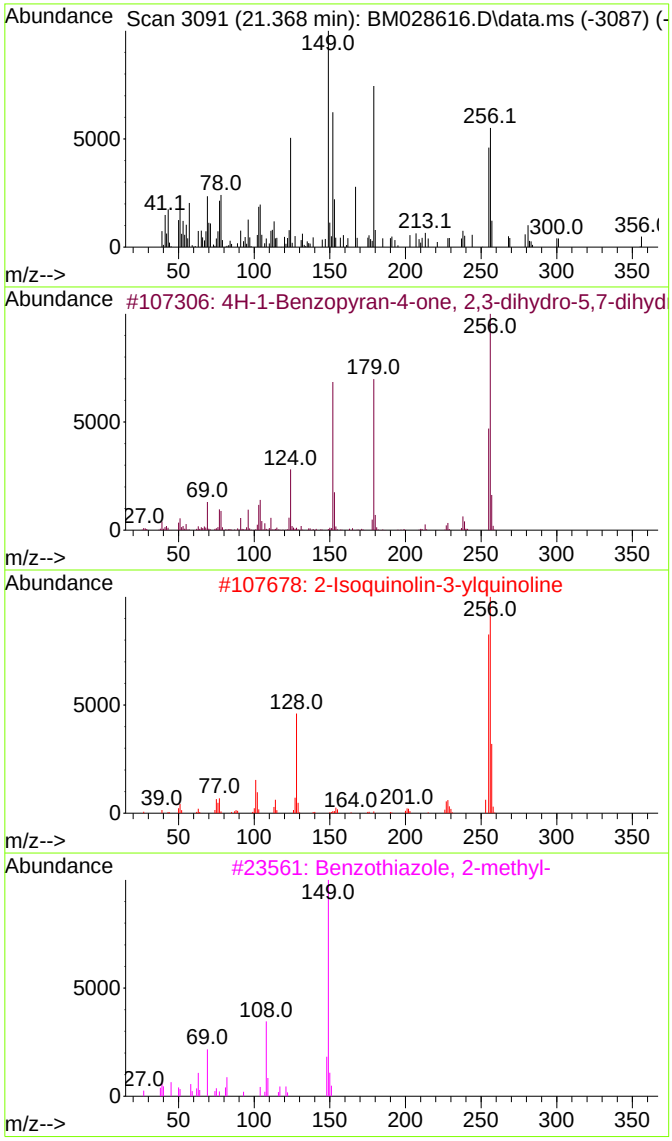
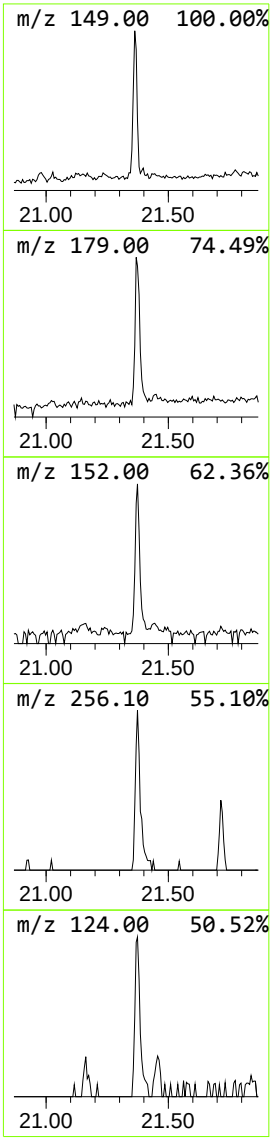
****

Peak Number 10 unknown21.368 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.368	2.51 ng	53631	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1-Benzopyran-4-one, 2,3-dihyd...	256	C15H12O4	000480-39-7	22
2	2-Isoquinolin-3-ylquinoline	256	C18H12N2	1000220-86-8	11
3	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	11
4	3-(4-(4-Fluorophenyl)-1,3-thiazo...	256	C14H9FN2S	1000298-16-6	11
5	O-Nitroacetophenone oxime	180	C8H8N2O3	010342-62-8	11





Tentatively Identified Compound (LSC) summary

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Data File : BM028616.D
Acq On : 29 Jan 2021 21:17
Operator : CG/JU
Sample : M1271-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR-200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.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
(S)-(+)-1,2-Pro...	3.534	5.0	ng	39035	1	7.928	156507	20.0
L-.alpha.-Terpi...	10.798	3.6	ng	39245	2	10.739	216221	20.0
n-Hexadecanoic ...	18.198	9.8	ng	150009	4	17.315	307776	20.0
Octadecanoic acid	19.462	2.9	ng	62292	5	21.456	427785	20.0
Benzene, 1,3-di...	20.068	2.3	ng	48557	5	21.456	427785	20.0
unknown20.221	20.221	2.1	ng	45347	5	21.456	427785	20.0
Acridin-9-amine...	20.456	3.7	ng	78326	5	21.456	427785	20.0
1-Phenanthrenec...	21.027	2.7	ng	57979	5	21.456	427785	20.0
1-Nonadecene	21.162	8.9	ng	190758	5	21.456	427785	20.0
unknown21.368	21.368	2.5	ng	53631	5	21.456	427785	20.0