LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020221\
Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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: BM028630.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	301	306	314	rBV	8142	11006	1.16%	0.144%
2	5.469	382	388	398	rBV	423966	599268	63.32%	7.861%
3	7.104	659	666	680	rBV	394558	612272	64.70%	8.032%
4	7.928	799	806	812	rVB	101704	155309	16.41%	2.037%
5	9.104	998	1006	1018	rBV	236748	396757	41.93%	5.205%
6	10.739	1277	1284	1290	rVB	128630	207390	21.91%	2.720%
7	11.745	1449	1455	1459	rBV2	8678	13400	1.42%	0.176%
8	13.098	1681	1685	1690	rVV	13905	18228	1.93%	0.239%
9	13.198	1692	1702	1710	rVB	542182	789442	83.42%	10.356%
10	13.386	1723	1734	1743	rBV5	12667	33487	3.54%	0.439%
11	13.904	1817	1822	1828	rBV4	6181	11074	1.17%	0.145%
12	13.992	1833	1837	1840	rVV2	10782	14707	1.55%	0.193%
13	14.039	1840	1845	1851	rVB2	24440	45385	4.80%	0.595%
14	14.304	1886	1890	1897	rBV4	7690	17417	1.84%	0.228%
15	14.404	1901	1907	1914	rVV8	12913	29619	3.13%	0.389%
16	14.463	1914	1917	1924	rVB	15177	21948	2.32%	0.288%
17	14.580	1931	1937	1943	rVB2	187042	275625	29.13%	3.616%
18	14.974	1999	2004	2009	rVB4	7652	12077	1.28%	0.158%
19	15.080	2020	2022	2028	rVB3	6170	9472	1.00%	0.124%
20	15.357	2063	2069	2073	rBV5	6835	11360	1.20%	0.149%
21	15.415	2074	2079	2083	rVB	14445	18171	1.92%	0.238%
22	15.621	2109	2114	2124	rBV3	12364	23910	2.53%	0.314%
23	15.815	2142	2147	2153	rVB	15775	26019	2.75%	0.341%
24	16.062	2180	2189	2197	rBV	395539	584994	61.82%	7.674%
25	16.292	2220	2228	2233	rBV	35870	71443	7.55%	0.937%
26	16.621	2277	2284	2289	rBV6	6734	14852	1.57%	0.195%
27	16.674	2289	2293	2301	rVB5	9108	14012	1.48%	0.184%
28	17.057	2354	2358	2362	rBV2	18372	24535	2.59%	0.322%
29	17.109	2363	2367	2377	rVB4	18265	41712	4.41%	0.547%
30	17.315	2396	2402	2406	rBV	196650	287954	30.43%	3.777%
31	17.357	2406	2409	2414	rVB	90049	115778	12.23%	1.519%
32	17.445	2419	2424	2430	rVB	23910	33583	3.55%	0.441%
33	17.792	2480	2483	2486	rBV	14353	15029	1.59%	0.197%
34	18.192	2544	2551	2555	rBV2	81323	130906	13.83%	1.717%
35	18.233	2555	2558	2565	rVV	38667	53367	5.64%	0.700%
36	18.309	2567	2571	2576	rVV2	11134	21081	2.23%	0.277%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020221\
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Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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	18.374	2577	2582	2586	rVV2	34204	65630	6.94%	0.861%
38	18.415	2586	2589	2596	rVB	15600	22282	2.35%	0.292%
39	18.480	2596	2600	2604	rBV	10733	13297	1.41%	0.174%
40	18.680	2630	2634	2637	rVB2	11846	14910	1.58%	0.196%
41	18.921	2672	2675	2681	rBV2	7311	10762	1.14%	0.141%
42	18.974	2681	2684	2687	rBV	9950	11841	1.25%	0.155%
43	19.098	2700	2705	2710	rBV2	22019	41020	4.33%	0.538%
44	19.156	2710	2715	2718	rVV3	6517	11817	1.25%	0.155%
45	19.233	2724	2728	2732	rBV2	6878	12803	1.35%	0.168%
46	19.356	2744	2749	2755	rVB	117668	151207	15.98%	1.983%
47	19.462	2762	2767	2772	rBV4	24229	36784	3.89%	0.483%
48	19.686	2801	2805	2806	rBV	19449	21620	2.28%	0.284%
49	19.715	2806	2810	2818	rVV	143263	207069	21.88%	2.716%
50	19.786	2819	2822	2828	rVB2	8848	12946	1.37%	0.170%
51	19.915	2839	2844	2849	rBV	795393	946349	100.00%	12.414%
52	20.045	2860	2866	2872	rBV3	11785	28520	3.01%	0.374%
53	20.209	2884	2894	2899	rBV2	34197	69462	7.34%	0.911%
54	20.309	2907	2911	2916	rBV	26069	37781	3.99%	0.496%
55	20.362	2916	2920	2924	rBV	27663	36509	3.86%	0.479%
56	20.503	2940	2944	2947	rBV2	20856	26349	2.78%	0.346%
57	20.550	2948	2952	2956	rVV	16868	22179	2.34%	0.291%
58	21.109	3045	3047	3051	rBV2	8931	11962	1.26%	0.157%
59	21.162	3051	3056	3067	rVV3	116206	173345	18.32%	2.274%
60	21.456	3100	3106	3110	rBV2	276322	423234	44.72%	5.552%
61	21.492	3110	3112	3119	rVB	56766	71540	7.56%	0.938%
62	23.615	3470	3473	3481	rVB	41113	71034	7.51%	0.932%
63	23.715	3484	3490	3496	rBV2	164782	308458	32.59%	4.046%

Sum of corrected areas: 7623299

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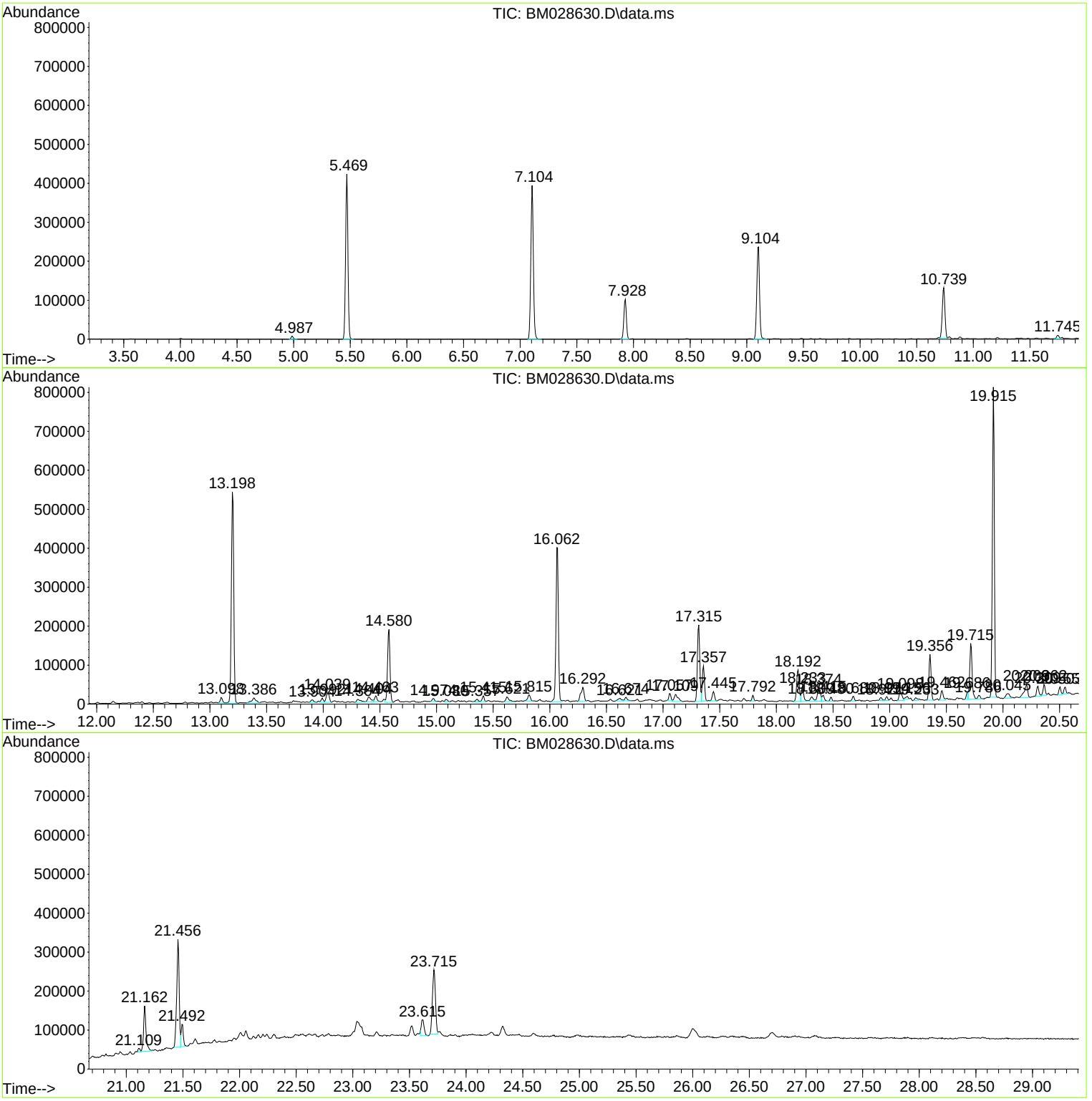
Instrument :
BNA_M
ClientSampleId :
JJ_BH_02_4-6

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

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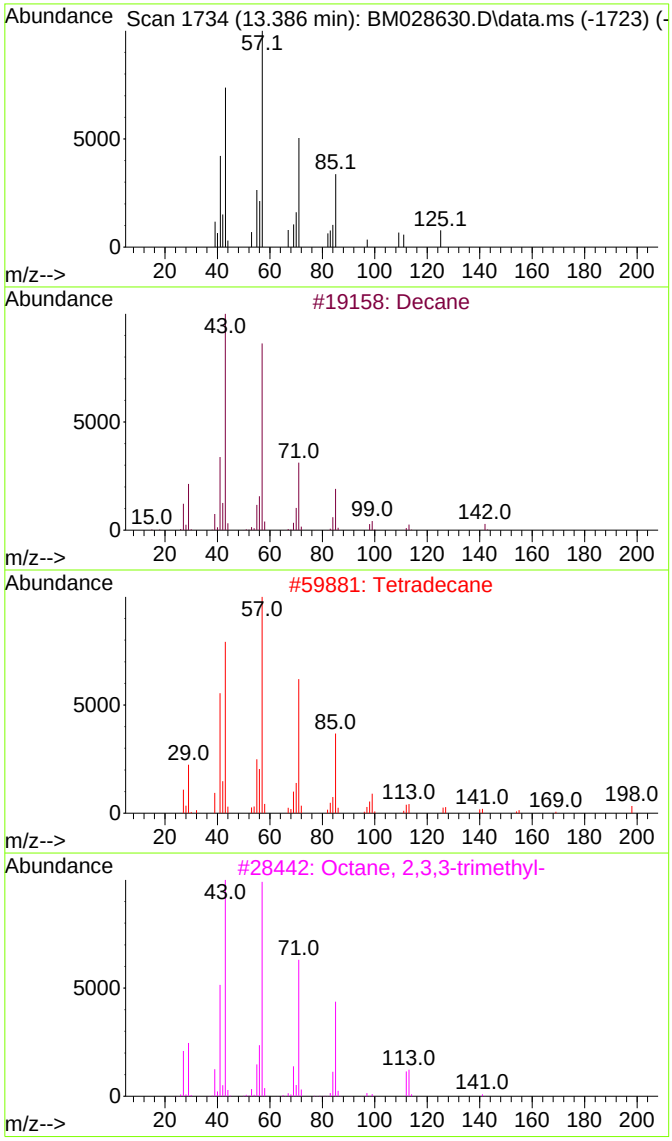
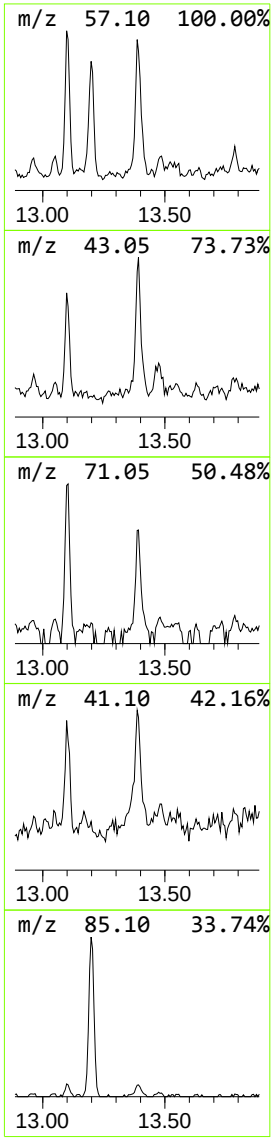
Peak Number 1 Decane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.386	2.43 ng	33487	Acenaphthene-d10	14.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	72
2	Tetradecane	198	C14H30	000629-59-4	72
3	Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	64
4	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	59
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59





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Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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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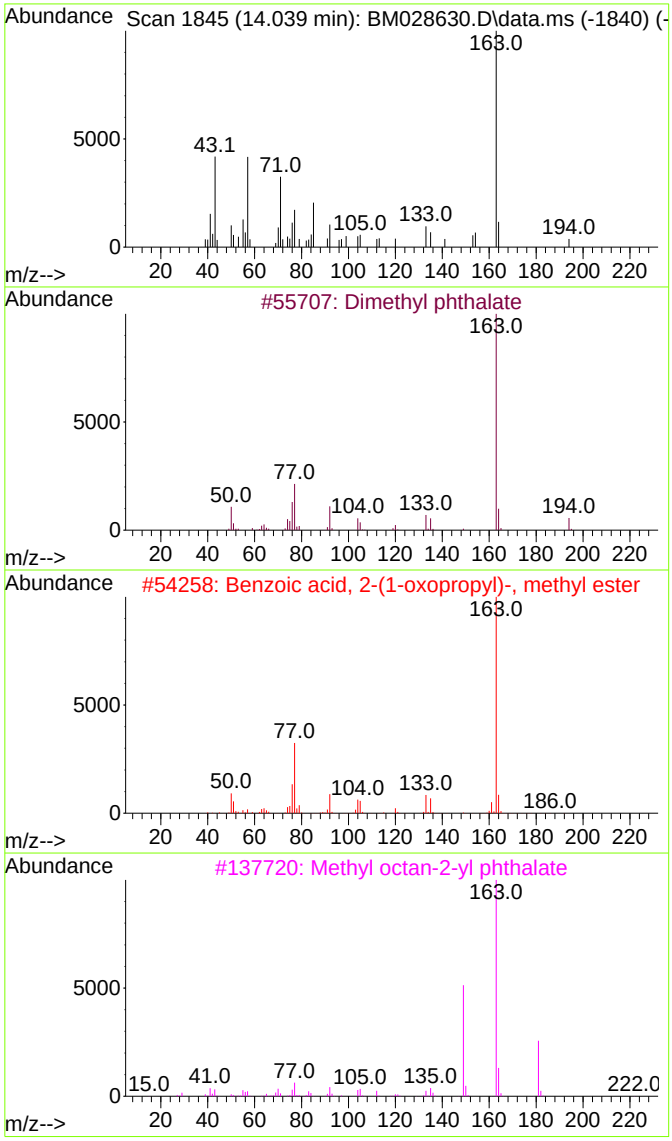
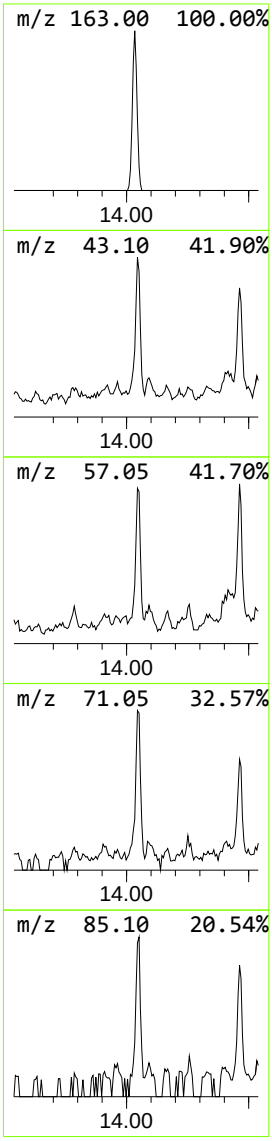
Peak Number 2 Benzoic acid, 2-(1-oxopropy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	3.29 ng	45385	Acenaphthene-d10	14.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl phthalate	194	C10H10O4	000131-11-3	92
2	Benzoic acid, 2-(1-oxopropyl)-, ...	192	C11H12O3	032025-37-9	50
3	Methyl octan-2-yl phthalate	292	C17H24O4	1000373-81-2	50
4	1,2-Benzenedicarboxylic acid, bu...	236	C13H16O4	034006-76-3	50
5	Allyl methyl phthalate	220	C12H12O4	1000373-89-1	50





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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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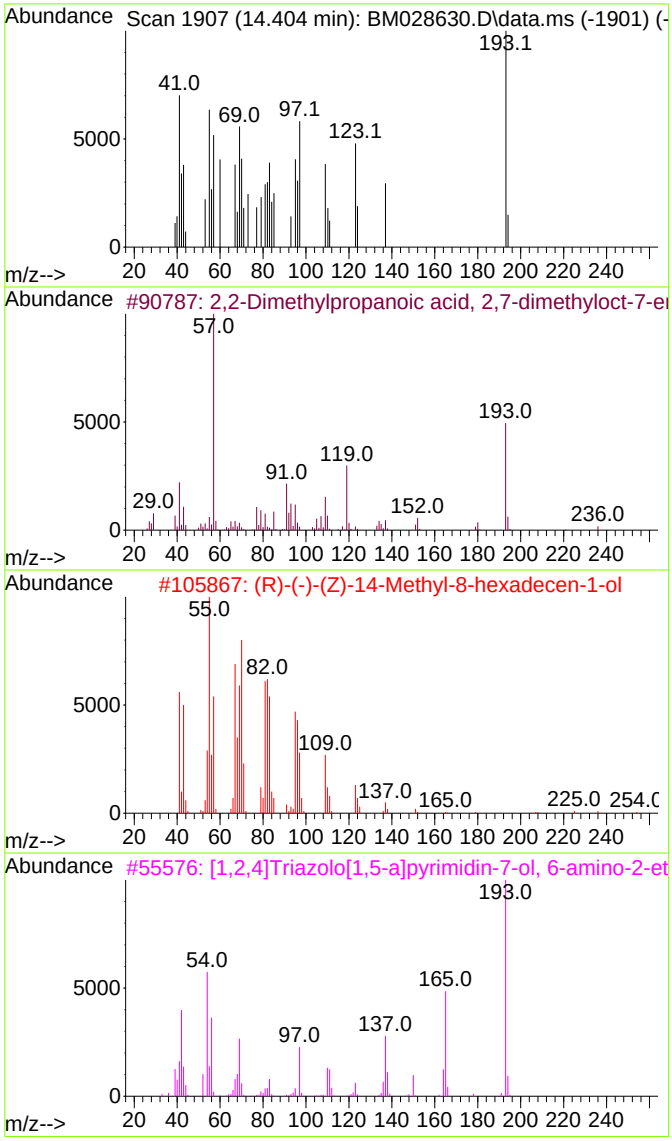
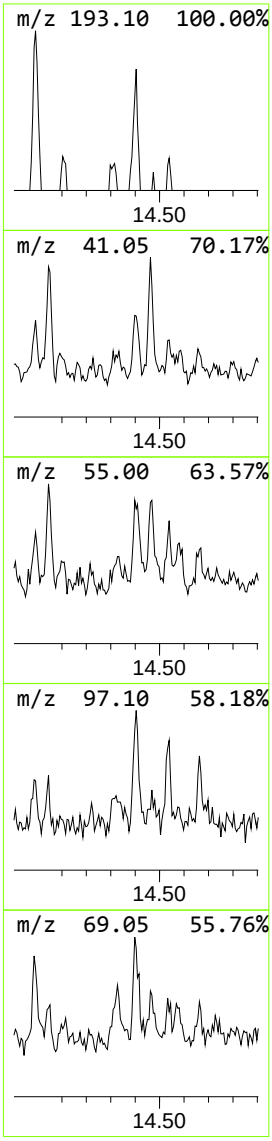
Peak Number 3 unknown14.404 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.404	2.15 ng	29619	Acenaphthene-d10	14.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylpropanoic acid, 2,7-...	236	C15H24O2	1000299-33-5	32
2	(R)-(-)-(Z)-14-Methyl-8-hexadece...	254	C17H34O	030689-78-2	27
3	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000351-50-1	25
4	2-(1-Butyl-2-nitroallyl)cyclohex...	239	C13H21NO3	1000192-05-9	25
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-97-1	11





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Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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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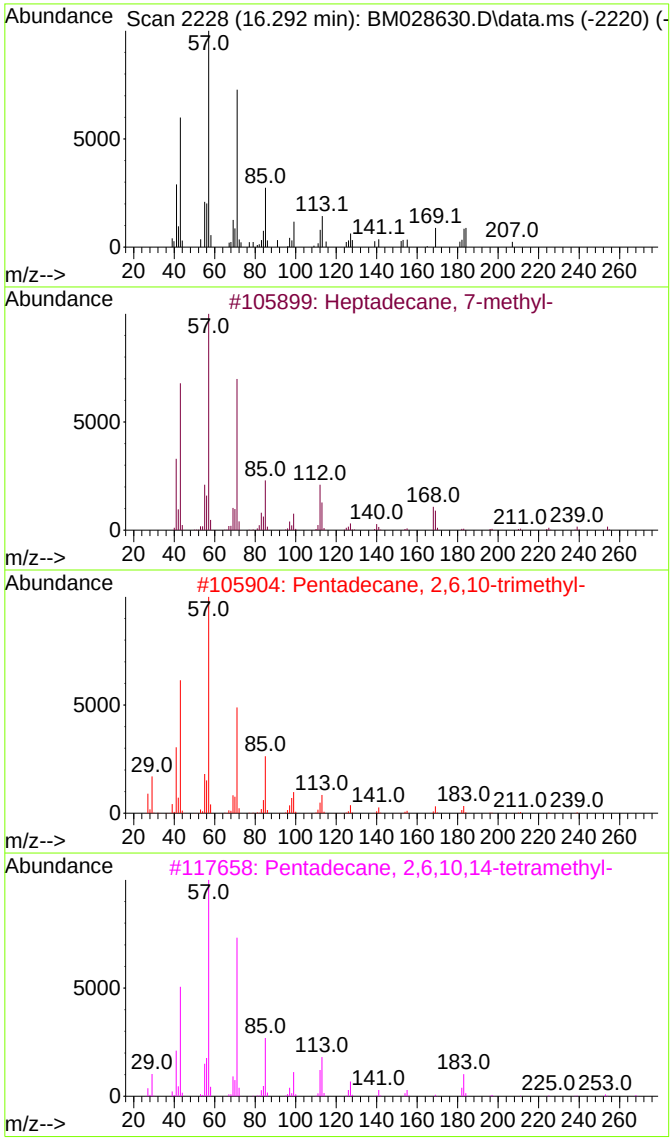
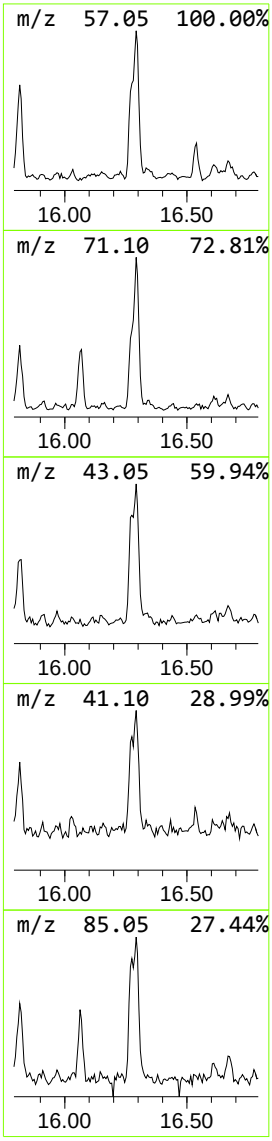
Peak Number 4 Heptadecane, 7-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.292	4.96 ng	71443	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	86
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80
4	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	74
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72





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Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JJ_BH_02_4-6

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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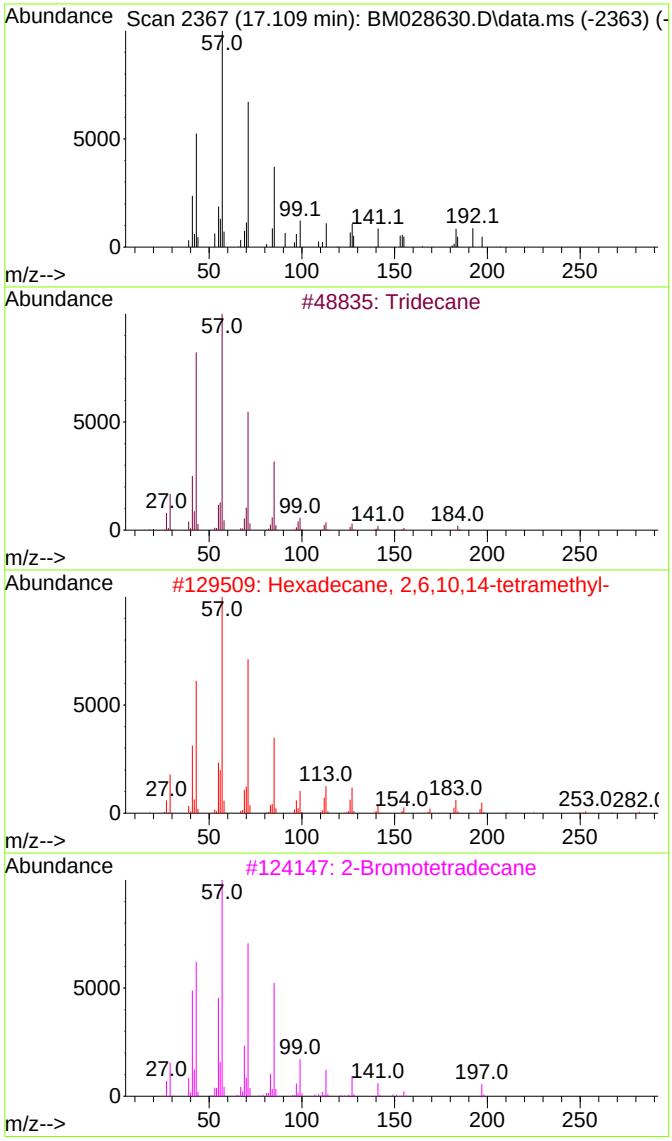
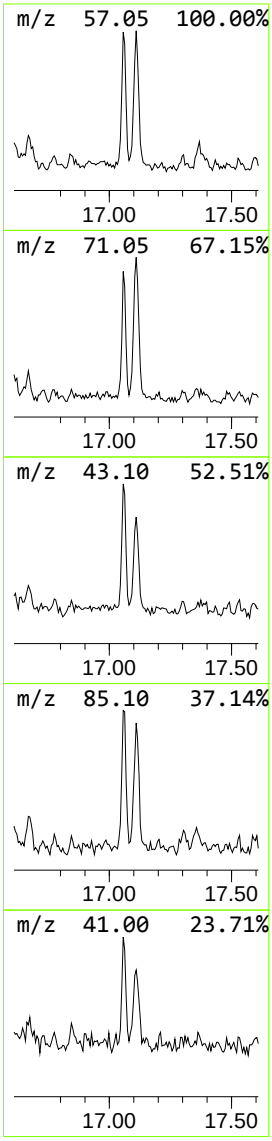
Peak Number 5 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.110	2.90 ng	41712	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	83
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	72
4	Octadecane	254	C18H38	000593-45-3	72
5	Heptacosane	380	C27H56	000593-49-7	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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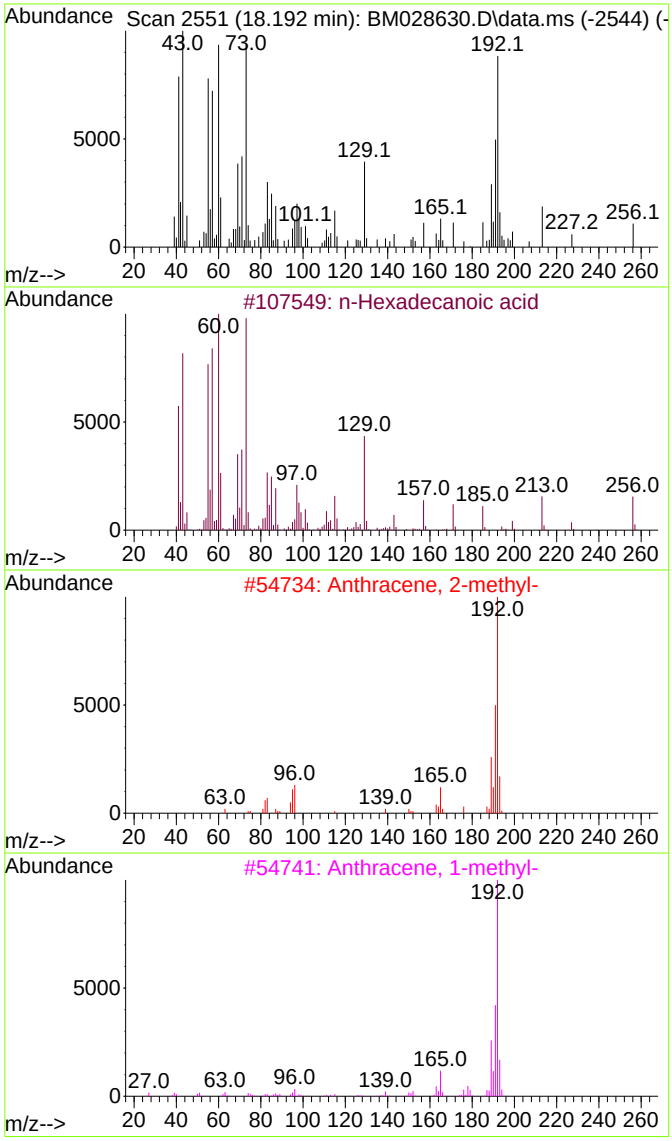
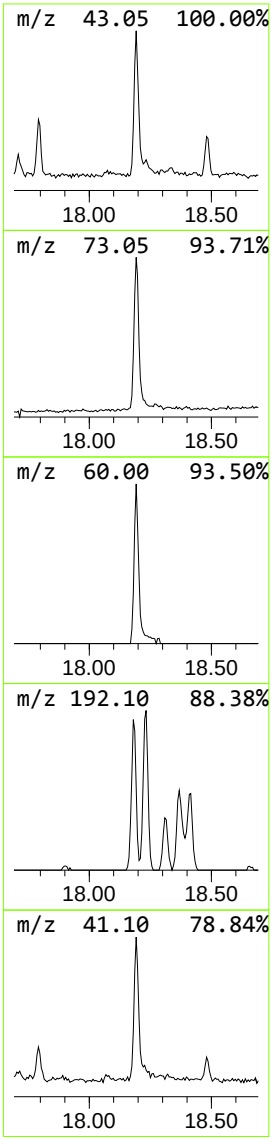
Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	9.09 ng	130906	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	62
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	60





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Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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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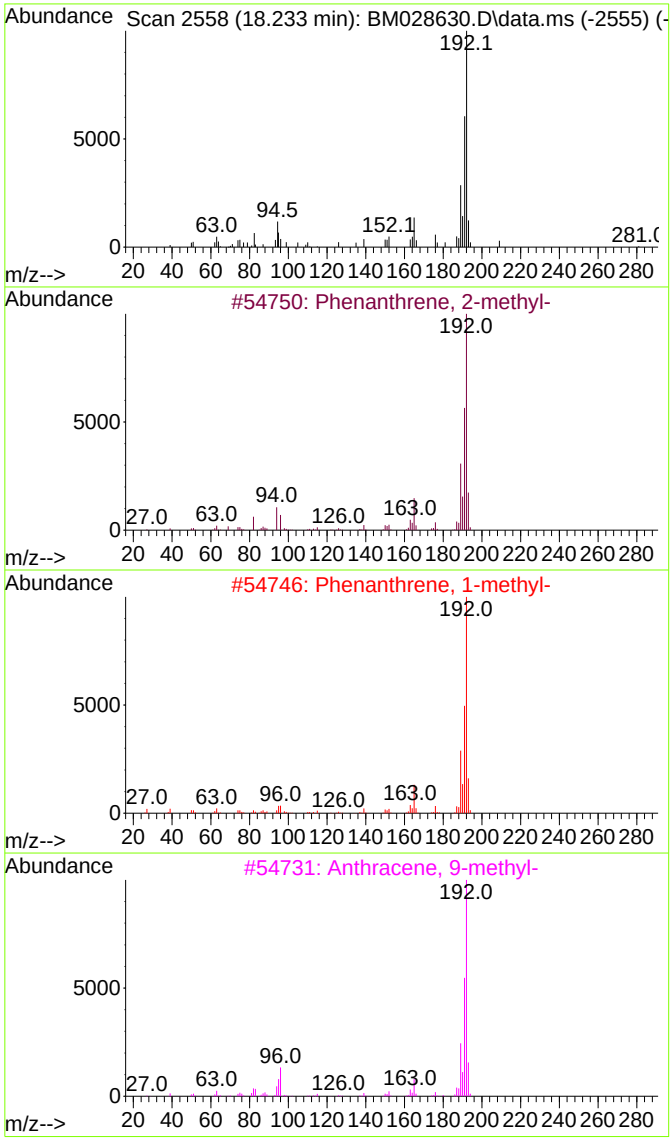
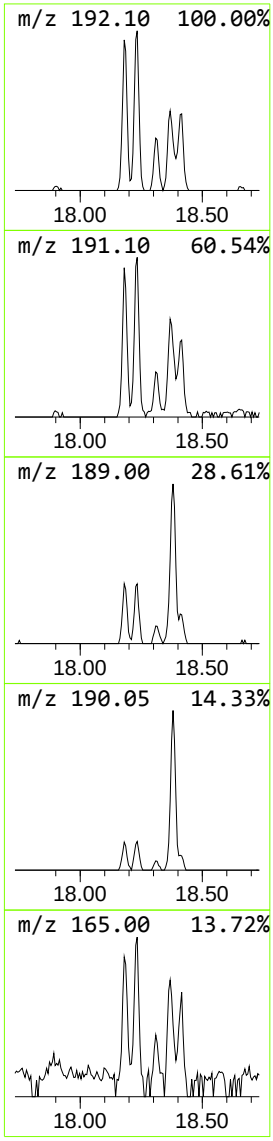
Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	3.71 ng	53367	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	81





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Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

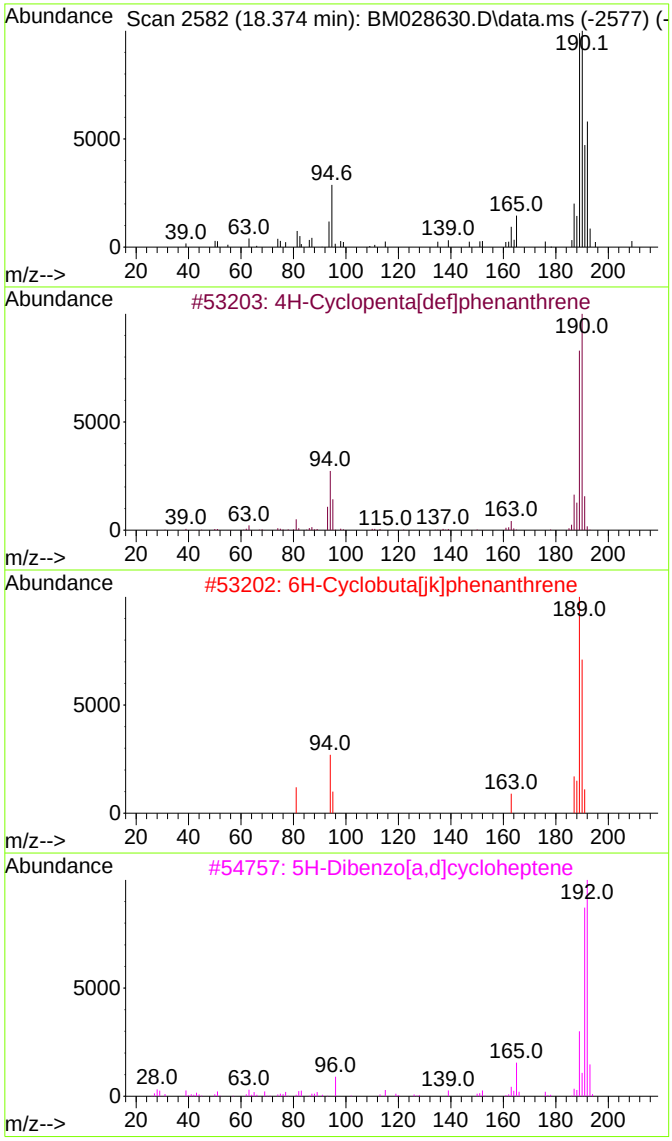
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

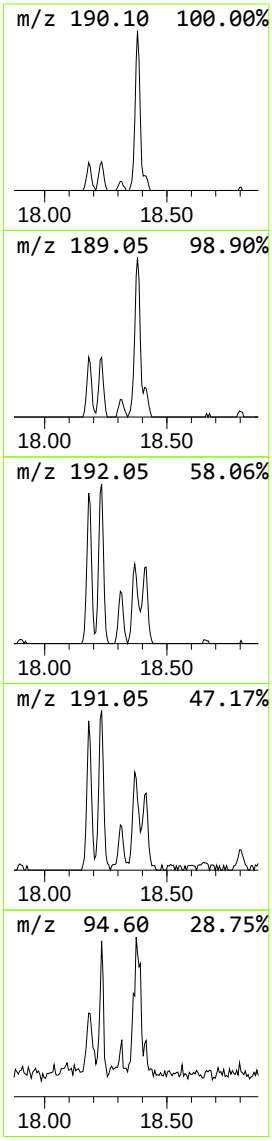
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	4.56 ng	65630	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
4	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	38
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30





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Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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

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TIC Integration Parameters: LSCINT.P

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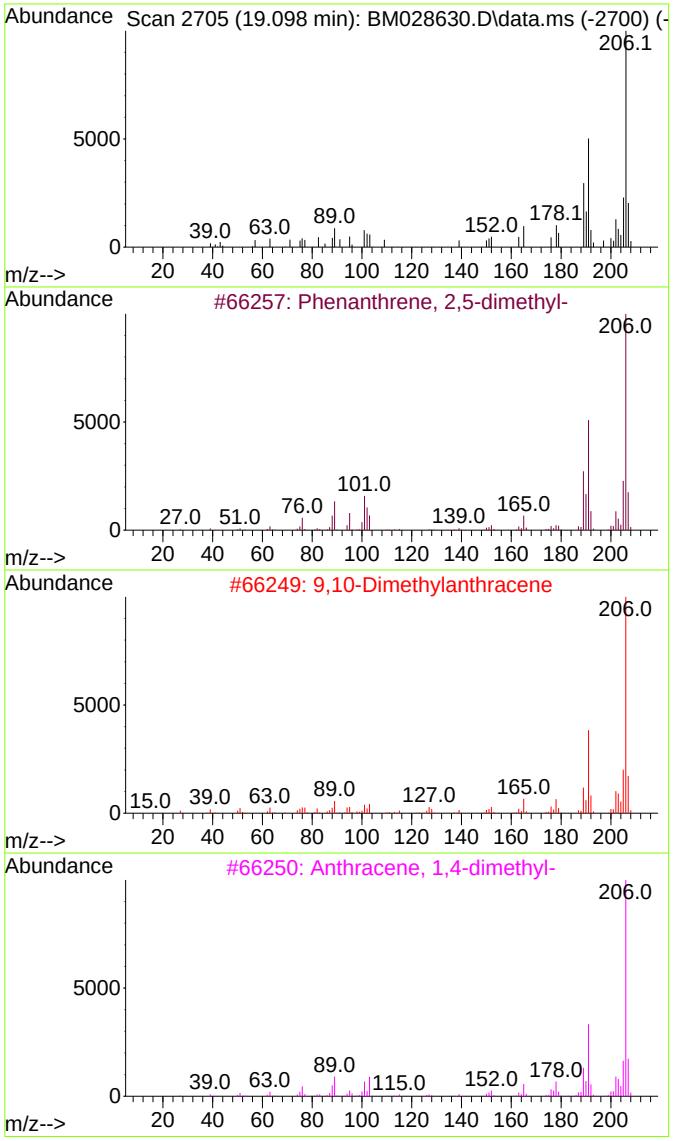
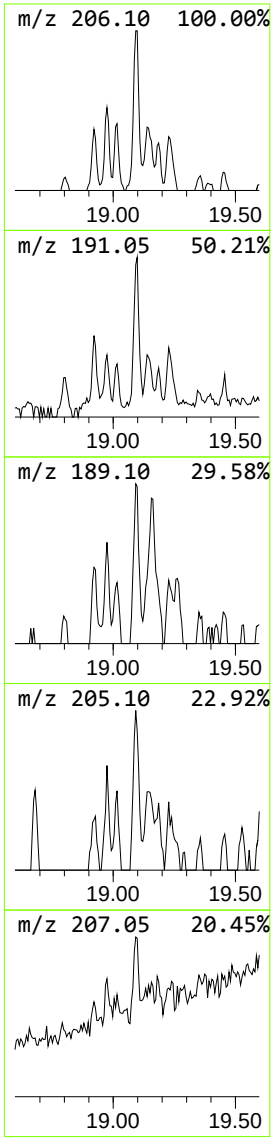
Peak Number 9 Phenanthrene, 2,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.098	2.85 ng	41020	Phenanthrene-d10	17.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	95
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90
5	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	81





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Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JJ_BH_02_4-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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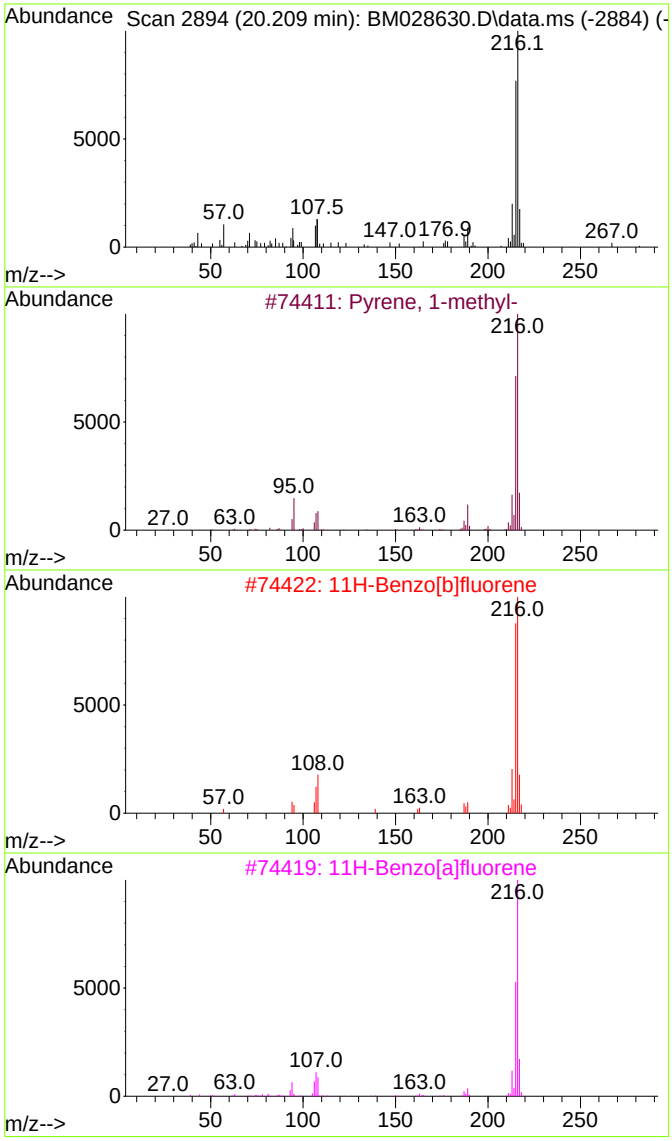
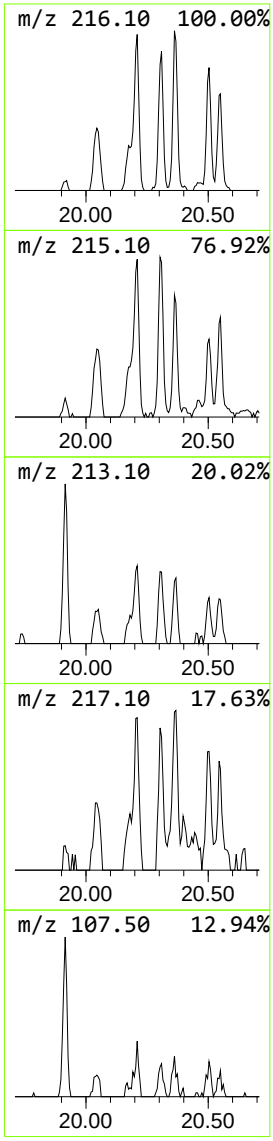
Peak Number 10 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.209	3.28 ng	69462	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020221\
Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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

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TIC Integration Parameters: LSCINT.P

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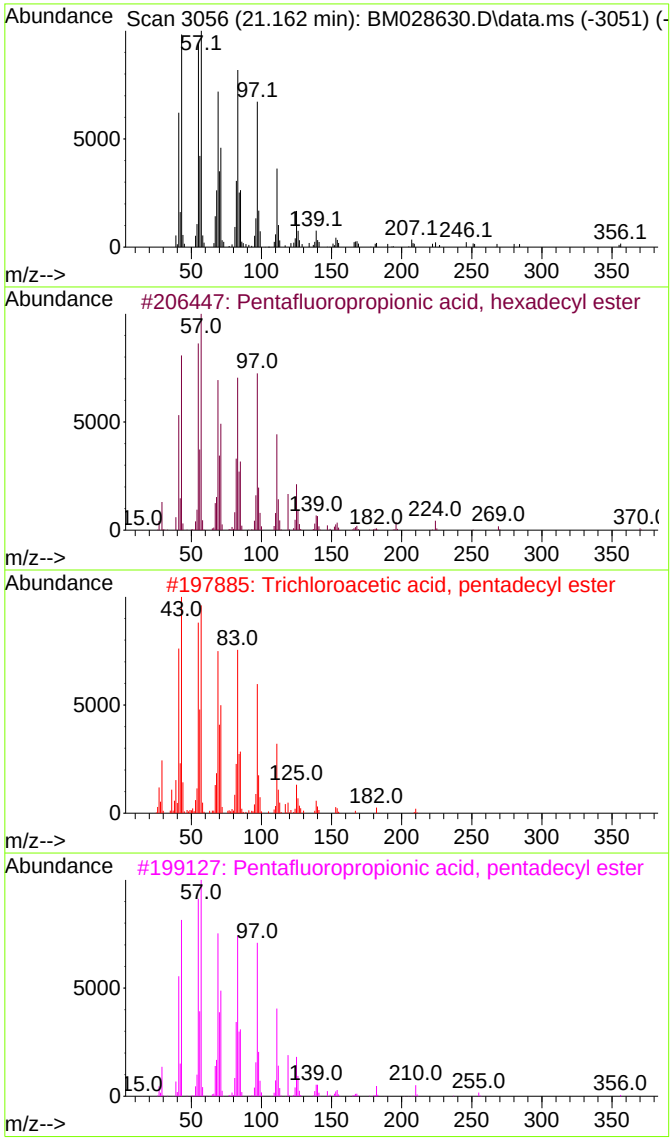
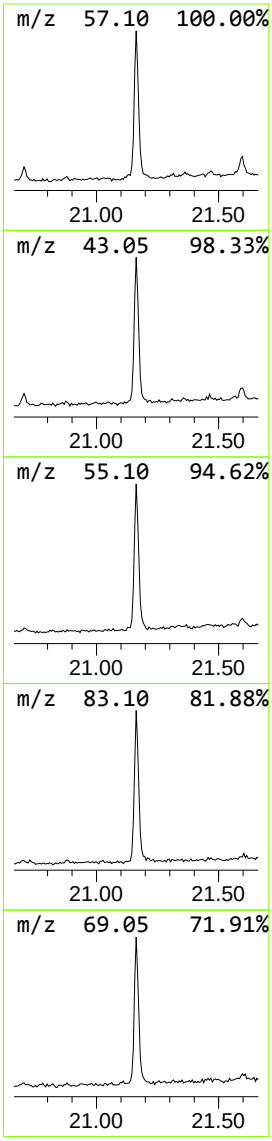
Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	8.19 ng	173345	Chrysene-d12	21.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020221\
Data File : BM028630.D
Acq On : 02 Feb 2021 19:48
Operator : CG/JU
Sample : M1286-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JJ_BH_02_4-6

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
Decane	13.386	2.4	ng	33487	3	14.580	275625	20.0
Benzoic acid, 2...	14.039	3.3	ng	45385	3	14.580	275625	20.0
unknown14.404	14.404	2.1	ng	29619	3	14.580	275625	20.0
Heptadecane, 7-...	16.292	5.0	ng	71443	4	17.315	287954	20.0
Tridecane	17.110	2.9	ng	41712	4	17.315	287954	20.0
n-Hexadecanoic ...	18.192	9.1	ng	130906	4	17.315	287954	20.0
Phenanthrene, 2...	18.233	3.7	ng	53367	4	17.315	287954	20.0
4H-Cyclopenta[d...	18.374	4.6	ng	65630	4	17.315	287954	20.0
Phenanthrene, 2...	19.098	2.9	ng	41020	4	17.315	287954	20.0
Pyrene, 1-methyl-	20.209	3.3	ng	69462	5	21.456	423234	20.0
Pentafluoroprop...	21.162	8.2	ng	173345	5	21.456	423234	20.0