LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051019\
Data File : BM020252.D
Acq On : 10 May 2019 23:06
Operator : JU/SJ
Sample : K2754-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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	5.357	396	403	412	rBV	2097832	3020254	52.78%	6.676%
2	6.946	665	673	687	rBV	2033319	3346668	58.48%	7.398%
3	7.304	726	734	750	rBV	2060935	3425912	59.87%	7.573%
4	7.775	807	814	821	rBV	452565	724438	12.66%	1.601%
5	8.093	860	868	877	rBV	1547558	2452422	42.86%	5.421%
6	8.940	1004	1012	1026	rBV	1176549	2032652	35.52%	4.493%
7	10.569	1281	1289	1298	rBV	569699	958976	16.76%	2.120%
8	13.033	1701	1708	1722	rBV	3206737	4747281	82.96%	10.494%
9	13.875	1845	1851	1858	rBV	249529	352437	6.16%	0.779%
10	14.416	1937	1943	1951	rBV2	880670	1332664	23.29%	2.946%
11	15.910	2191	2197	2211	rBV	2661443	3855418	67.37%	8.522%
12	16.133	2228	2235	2241	rBV2	33994	71720	1.25%	0.159%
13	17.168	2404	2411	2414	rBV	1098361	1583341	27.67%	3.500%
14	17.210	2414	2418	2425	rVV	512417	741861	12.96%	1.640%
15	17.298	2428	2433	2441	rVB	107236	167065	2.92%	0.369%
16	18.045	2555	2560	2564	rBV2	269009	404064	7.06%	0.893%
17	18.086	2564	2567	2575	rVB	78148	123046	2.15%	0.272%
18	18.233	2587	2592	2597	rBV3	106124	179684	3.14%	0.397%
19	18.545	2640	2645	2648	rBV	46332	60550	1.06%	0.134%
20	18.968	2711	2717	2721	rBV5	27887	62255	1.09%	0.138%
21	19.104	2736	2740	2745	rBV3	32908	61819	1.08%	0.137%
22	19.227	2755	2761	2768	rBV	1155338	1588068	27.75%	3.510%
23	19.327	2774	2778	2782	rBV4	63991	92413	1.61%	0.204%
24	19.468	2799	2802	2812	rVB2	37647	76695	1.34%	0.170%
25	19.557	2812	2817	2818	rBV	157589	213162	3.73%	0.471%
26	19.586	2818	2822	2830	rVB	935591	1343000	23.47%	2.969%
27	19.792	2850	2857	2871	rVB	4835021	5722395	100.00%	12.649%
28	19.904	2872	2876	2884	rVB3	41508	99916	1.75%	0.221%
29	20.086	2903	2907	2911	rVB	156586	214060	3.74%	0.473%
30	20.180	2920	2923	2927	rBV	102628	127176	2.22%	0.281%
31	20.586	2989	2992	2995	rVB	57278	59511	1.04%	0.132%
32	20.998	3059	3062	3065	rBV	62641	71562	1.25%	0.158%
33	21.051	3066	3071	3080	rVV5	285508	506810	8.86%	1.120%
34	21.351	3115	3122	3126	rBV2	1088267	2008124	35.09%	4.439%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051019\
Data File : BM020252.D
Acq On : 10 May 2019 23:06
Operator : JU/SJ
Sample : K2754-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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	21.386	3126	3128	3134	rVB	400673	462541	8.08%	1.022%
36	21.486	3142	3145	3146	rBV	90322	96939	1.69%	0.214%
37	22.392	3296	3299	3304	rBV	138046	177155	3.10%	0.392%
38	22.521	3318	3321	3326	rVB	137224	170239	2.97%	0.376%
39	22.909	3384	3387	3389	rBV2	100917	135962	2.38%	0.301%
40	22.945	3389	3393	3399	rVV	236214	480359	8.39%	1.062%
41	23.439	3473	3477	3482	rBV	156714	268933	4.70%	0.594%
42	23.539	3490	3494	3501	rVB	296379	516819	9.03%	1.142%
43	23.639	3505	3511	3517	rBV	566163	1101809	19.25%	2.436%

Sum of corrected areas: 45238175

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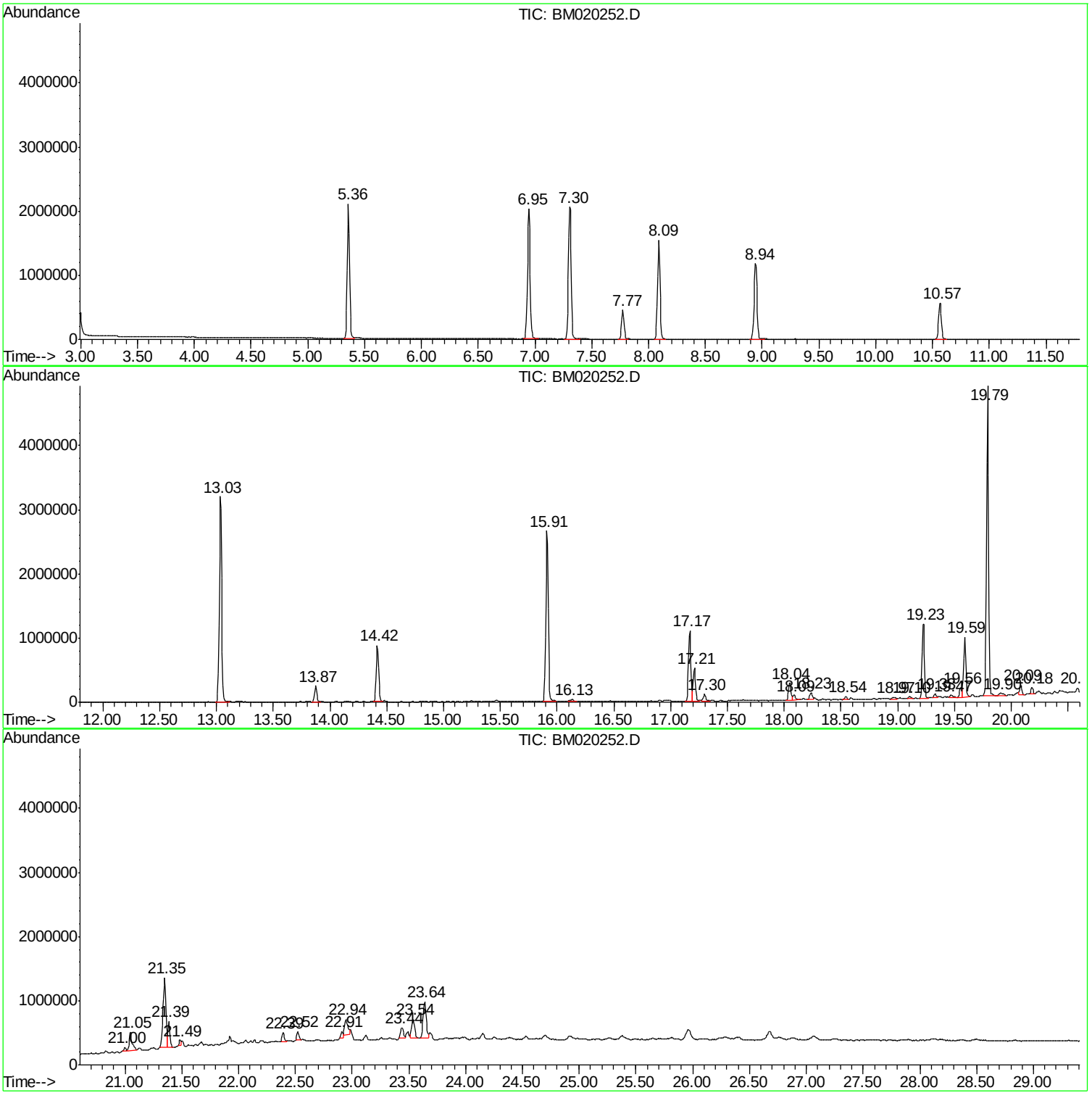
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BM020252.D
Acq On : 10 May 2019 23:06
Operator : JU/SJ
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ALS Vial : 6 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

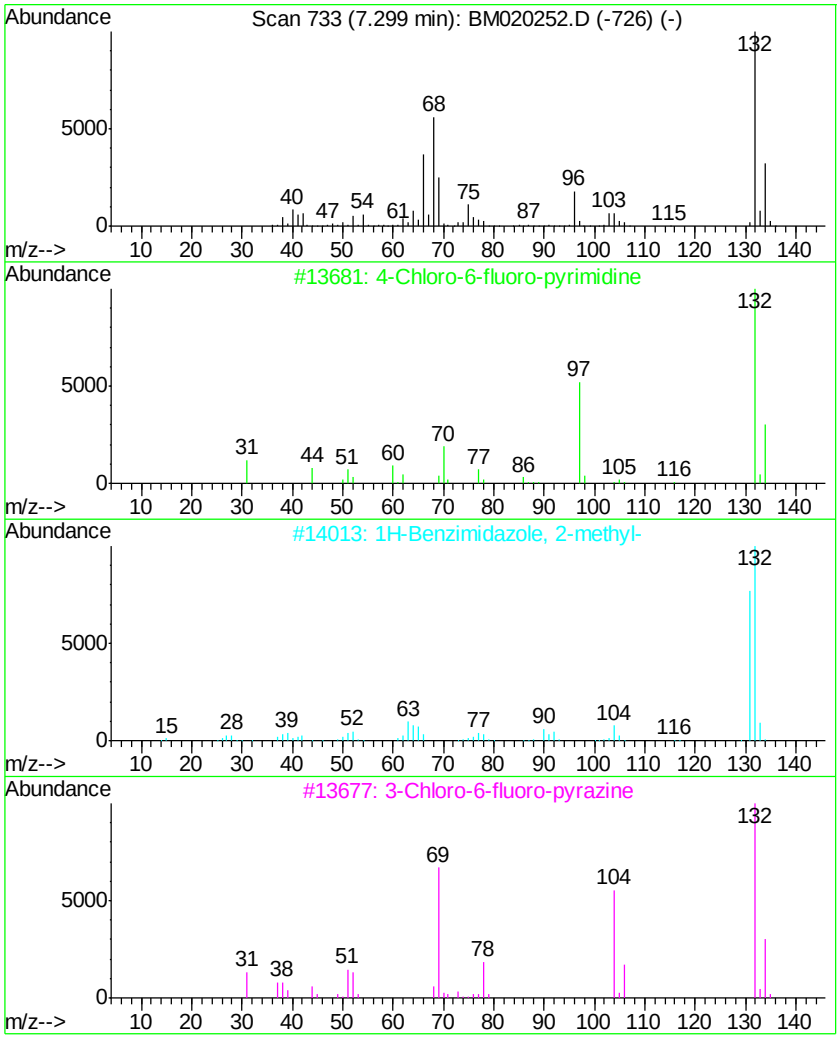
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

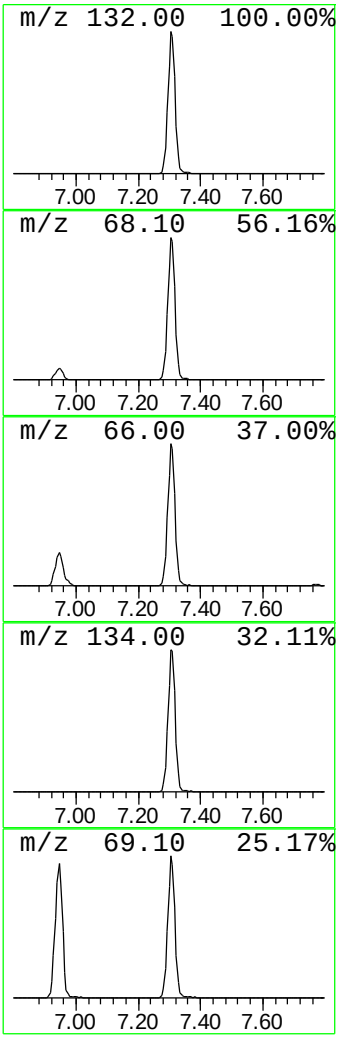
****

Peak Number 1 unknown7.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	94.58 ng	3425910	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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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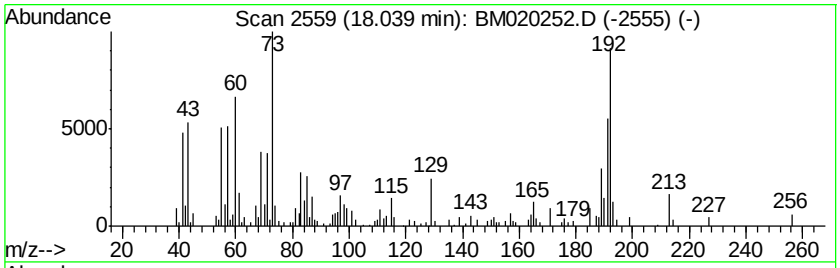
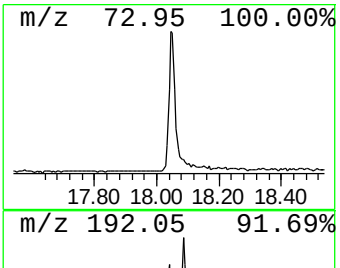
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	5.10 ng	404064	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
3	Tridecanoic acid	214	C13H26O2	000638-53-9	43
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Heptanoic acid	130	C7H14O2	000111-14-8	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051019\
Data File : BM020252.D
Acq On : 10 May 2019 23:06
Operator : JU/SJ
Sample : K2754-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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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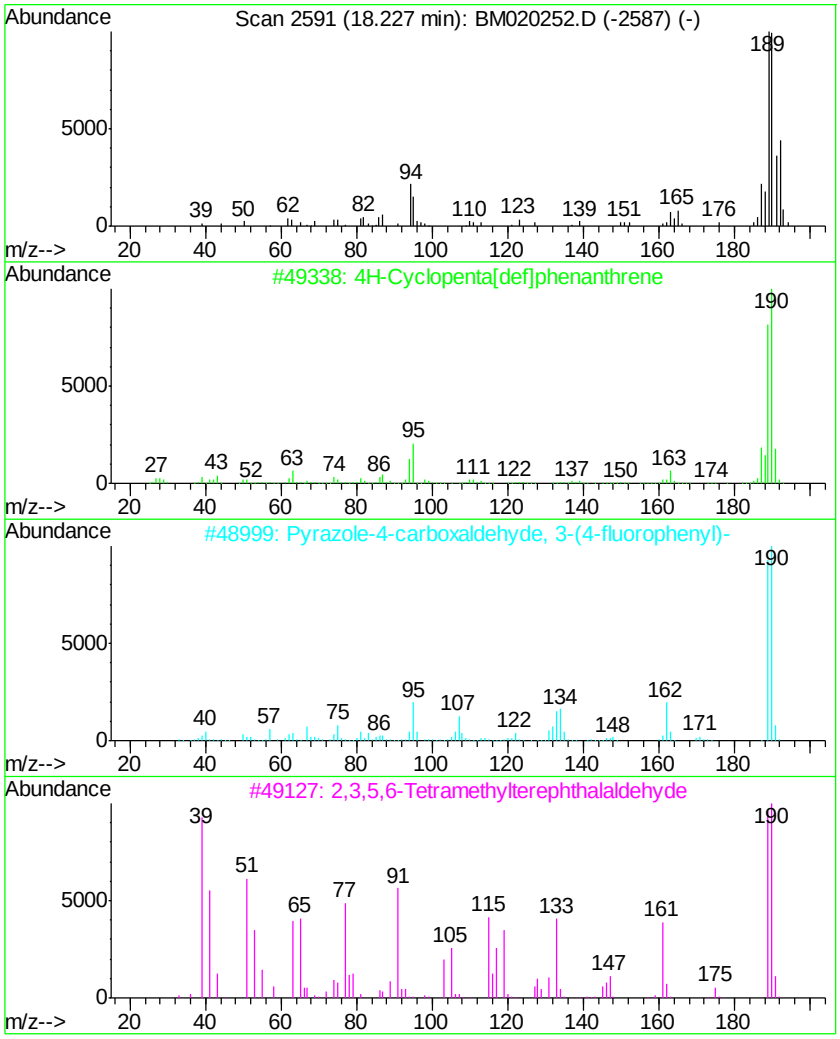
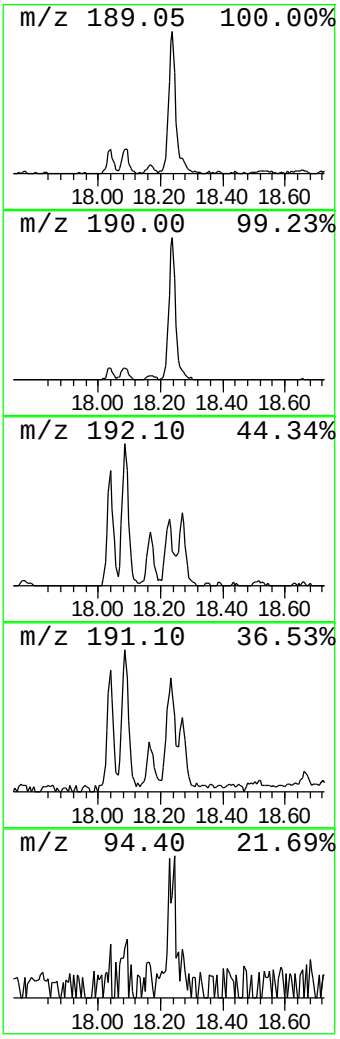
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	2.27 ng	179684	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	95
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	4-(4-Chlorophenyl)pyridine	189	C11H8ClN	005957-96-0	17





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : C-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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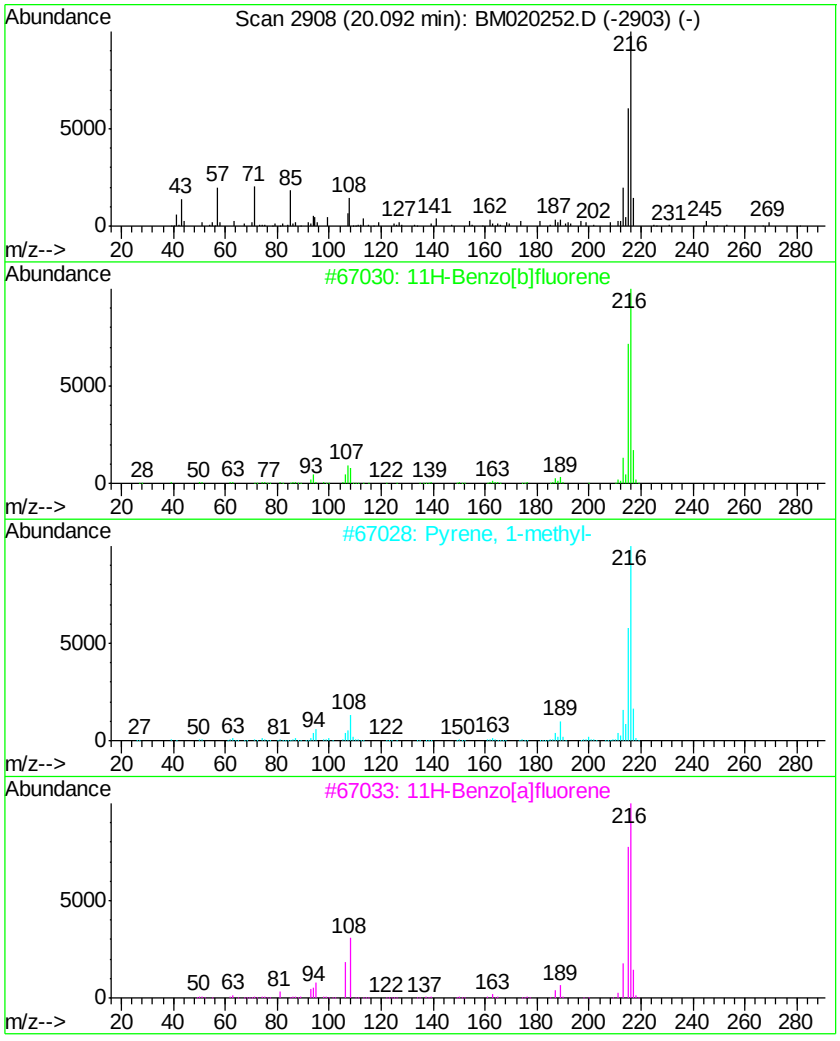
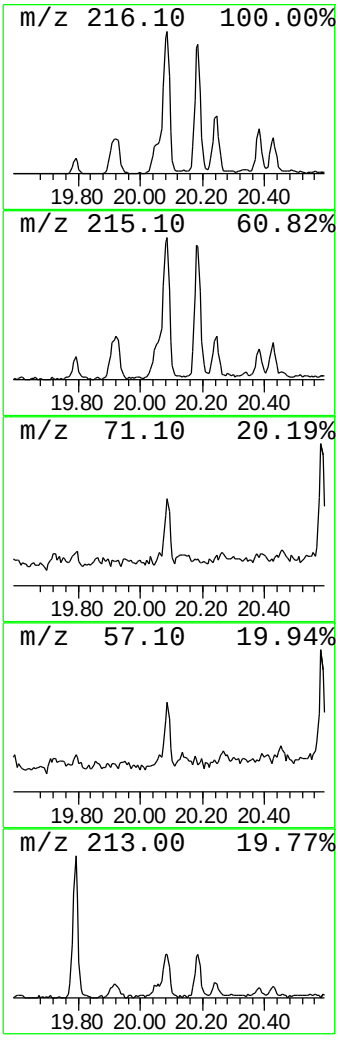
Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.09	2.13 ng	214060	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	80
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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
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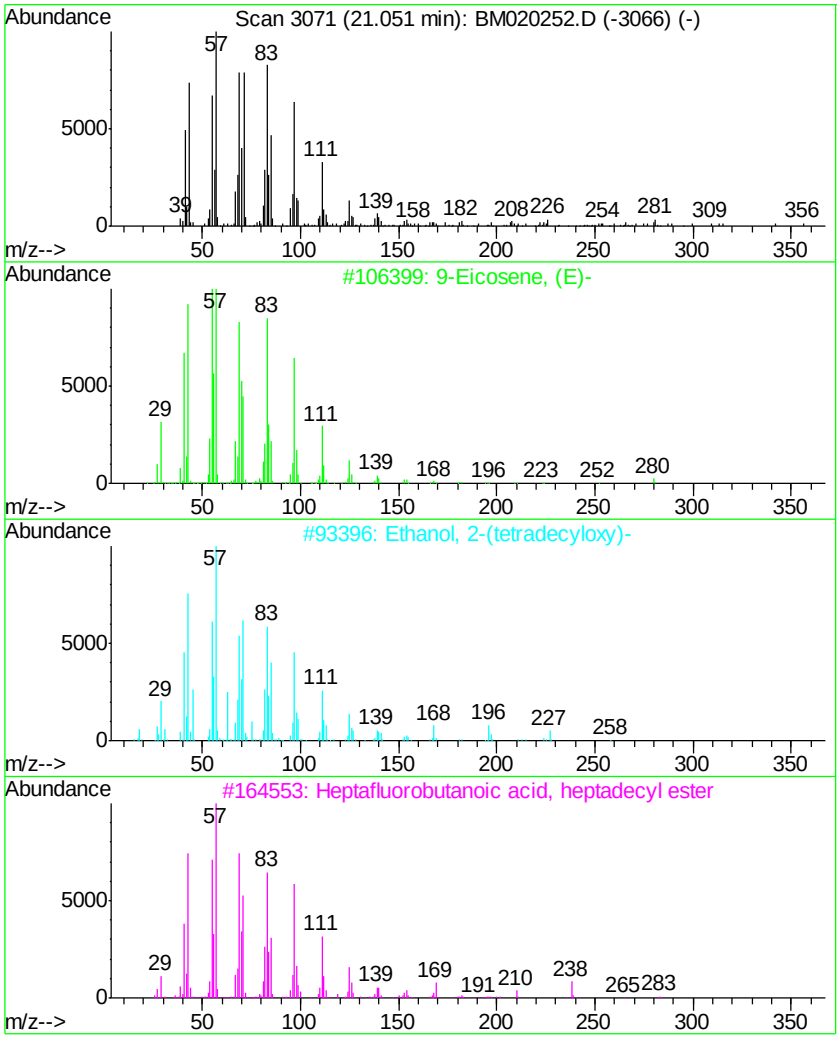
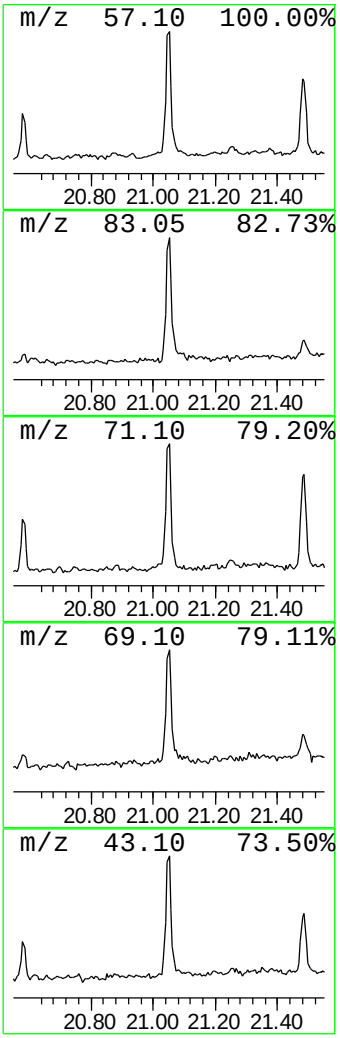
****

Peak Number 7 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	5.05 ng	506810	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	89
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	86
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	74
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	68





Library Search Compound Report

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Acq On : 10 May 2019 23:06
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Sample : K2754-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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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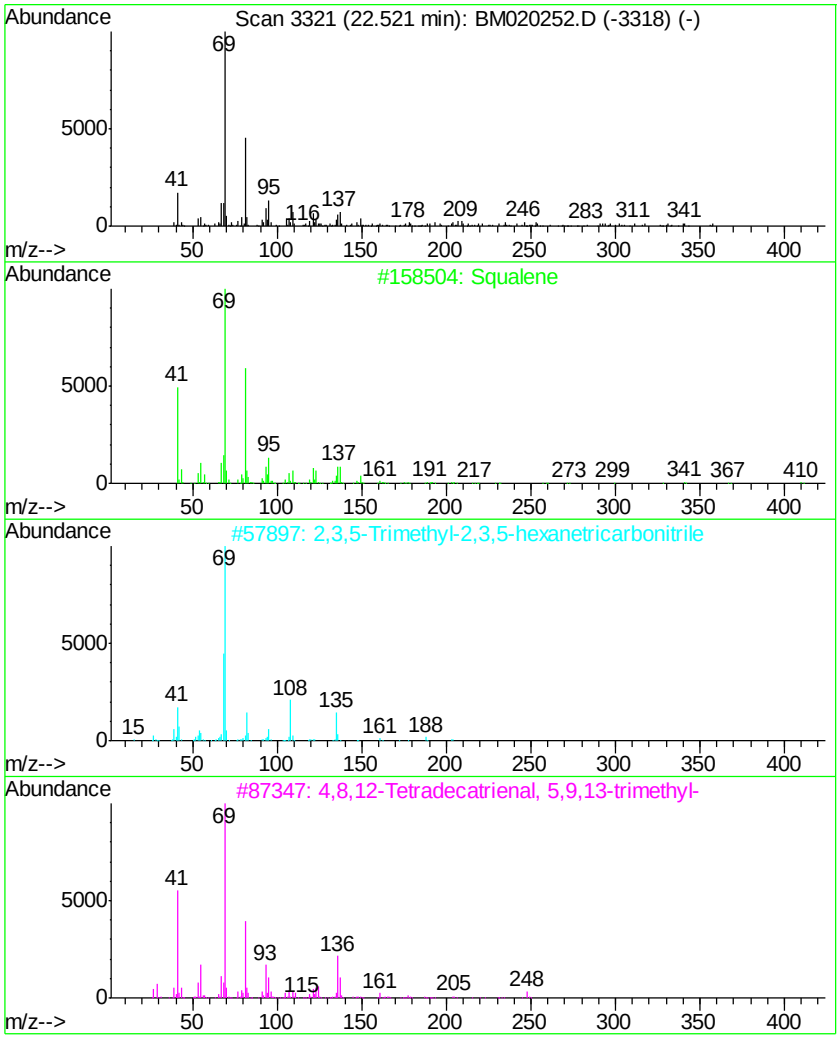
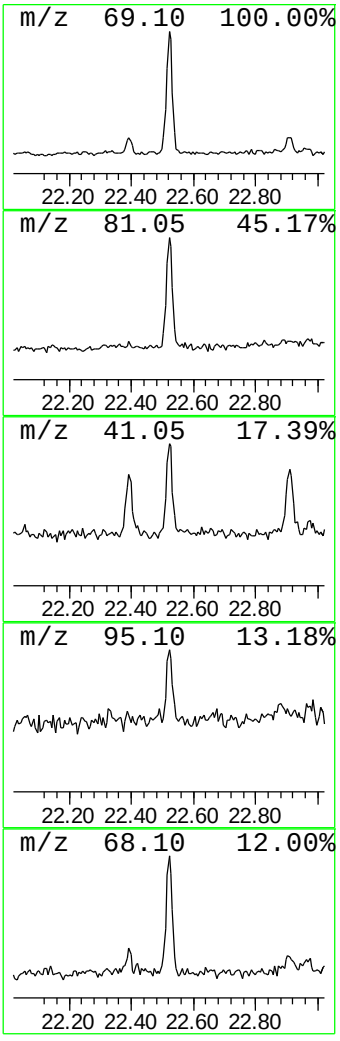
Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.52	3.09 ng	170239	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	74
2	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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

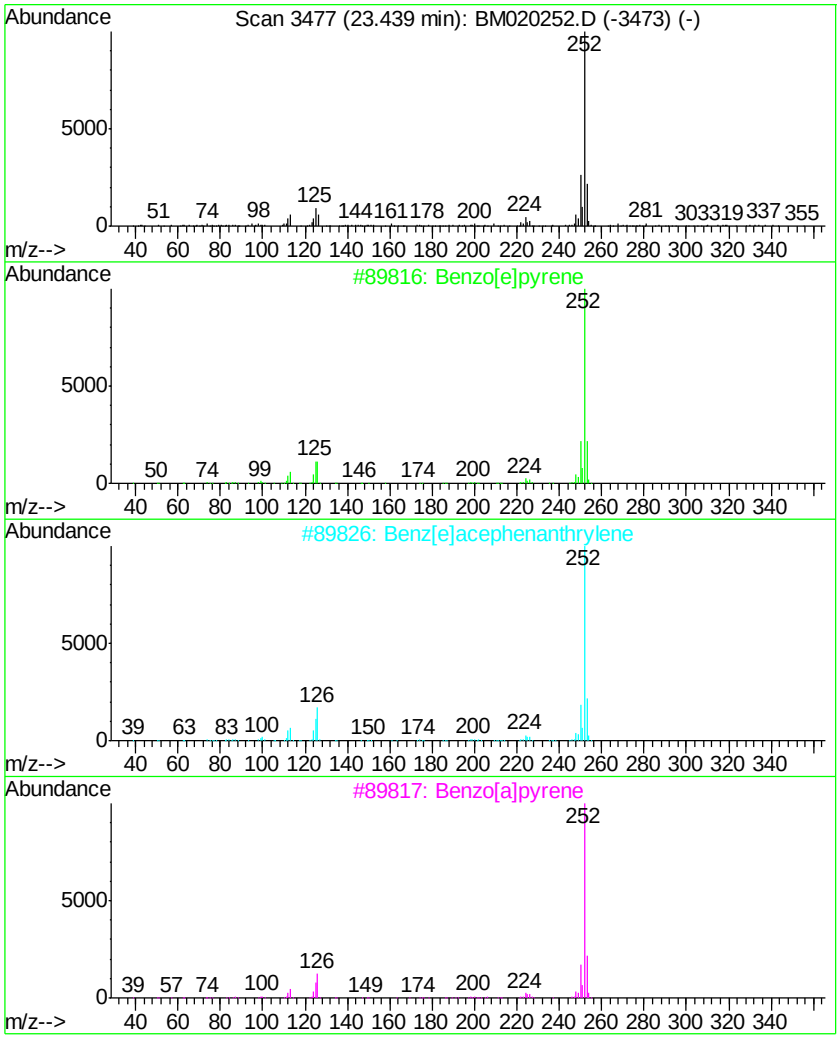
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

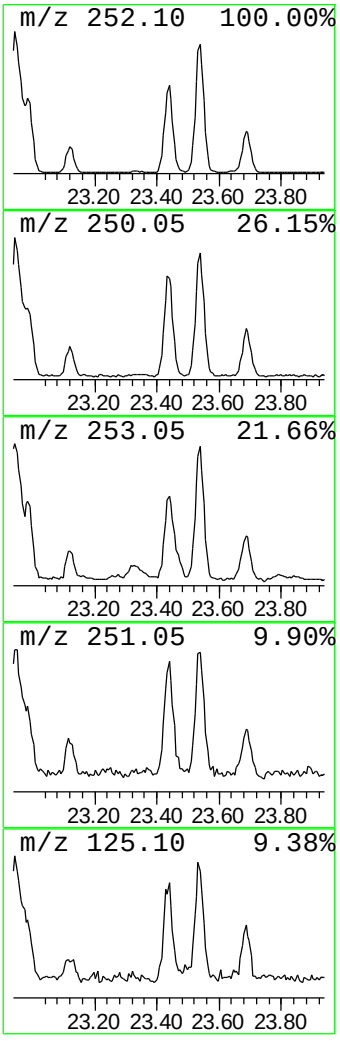
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.44	4.88 ng	268933	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Perylene	252	C20H12	000198-55-0	89
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051019\
Data File : BM020252.D
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Operator : JU/SJ
Sample : K2754-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C-1

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.30	7.30	94.6	ng	3425910	1	7.77	724438	20.0
n-Hexadecanoic acid	18.04	5.1	ng	404064	4	17.17	1583340	20.0
4H-Cyclopenta[def...	18.23	2.3	ng	179684	4	17.17	1583340	20.0
11H-Benzo[b]fluorene	20.09	2.1	ng	214060	5	21.35	2008120	20.0
9-Eicosene, (E)-	21.05	5.0	ng	506810	5	21.35	2008120	20.0
Squalene	22.52	3.1	ng	170239	6	23.64	1101810	20.0
Benzo[e]pyrene	23.44	4.9	ng	268933	6	23.64	1101810	20.0