LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : O2162-01
Misc :
ALS Vial : 19 Sample Multiplier: 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-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	284	292	302	rVB	1461565	1986910	24.84%	2.677%
2	5.475	365	372	383	rBV	3336270	4883875	61.07%	6.580%
3	7.081	638	645	662	rVB	3141310	4934617	61.70%	6.649%
4	7.910	777	786	794	rBV	915915	1460558	18.26%	1.968%
5	9.081	978	985	993	rBV	1933339	3131877	39.16%	4.220%
6	10.722	1252	1264	1270	rBV	1163358	2040274	25.51%	2.749%
7	10.775	1270	1273	1278	rVB	52655	81923	1.02%	0.110%
8	12.139	1496	1505	1509	rBV	46039	80877	1.01%	0.109%
9	12.386	1538	1547	1552	rVB2	66668	133452	1.67%	0.180%
10	12.604	1577	1584	1593	rBV2	61537	128970	1.61%	0.174%
11	13.186	1676	1683	1692	rBV	4281407	6379089	79.76%	8.595%
12	13.380	1711	1716	1722	rVB2	64910	109040	1.36%	0.147%
13	13.880	1796	1801	1806	rBV	84694	143063	1.79%	0.193%
14	14.280	1864	1869	1882	rBV	146046	248232	3.10%	0.334%
15	14.451	1894	1898	1904	rVB	94592	123194	1.54%	0.166%
16	14.557	1906	1916	1923	rBV	1651685	2527124	31.60%	3.405%
17	14.621	1923	1927	1934	rVB	209441	313067	3.91%	0.422%
18	14.957	1980	1984	1990	rVB	165195	246565	3.08%	0.332%
19	15.398	2053	2059	2063	rBV2	88309	127275	1.59%	0.171%
20	15.604	2089	2094	2099	rBV	289837	439293	5.49%	0.592%
21	15.915	2140	2147	2152	rVB2	247569	420287	5.26%	0.566%
22	16.051	2163	2170	2178	rBV	3341865	4799356	60.01%	6.467%
23	16.262	2202	2206	2208	rBV	116645	152286	1.90%	0.205%
24	16.609	2260	2265	2270	rVV2	77266	126381	1.58%	0.170%
25	16.662	2271	2274	2279	rVB2	70330	95247	1.19%	0.128%
26	16.762	2288	2291	2295	rVB3	62301	80672	1.01%	0.109%
27	16.962	2322	2325	2331	rVB3	60624	95003	1.19%	0.128%
28	17.057	2335	2341	2345	rVV2	138990	237808	2.97%	0.320%
29	17.127	2347	2353	2361	rVB2	178003	383260	4.79%	0.516%
30	17.309	2378	2384	2387	rBV	1929444	2718477	33.99%	3.663%
31	17.351	2387	2391	2398	rVV	1799110	2442371	30.54%	3.291%
32	17.439	2401	2406	2411	rVV	589862	801572	10.02%	1.080%
33	17.715	2449	2453	2459	rBV	108325	180513	2.26%	0.243%
34	17.798	2464	2467	2470	rBV	100019	109366	1.37%	0.147%
35	17.886	2479	2482	2490	rVB	85687	154181	1.93%	0.208%
36	18.204	2529	2536	2539	rBV2	800679	1452950	18.17%	1.958%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 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-BM032923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

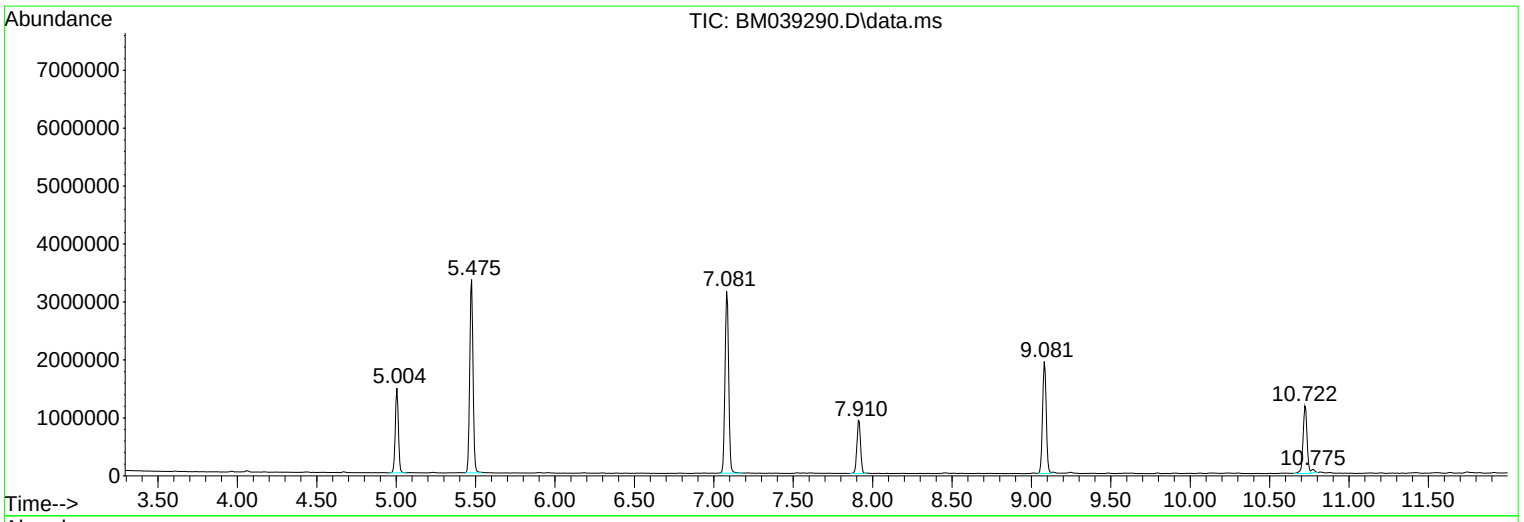
37	18.233	2539	2541	2547	rVV	444492	598057	7.48%	0.806%
38	18.315	2551	2555	2560	rVV	188693	287523	3.60%	0.387%
39	18.380	2561	2566	2570	rVV2	464511	875382	10.95%	1.179%
40	18.415	2570	2572	2580	rVB	217854	280232	3.50%	0.378%
41	18.492	2582	2585	2589	rBV	122309	154358	1.93%	0.208%
42	18.686	2614	2618	2622	rBV	182432	230582	2.88%	0.311%
43	18.980	2666	2668	2672	rVB	87101	80797	1.01%	0.109%
44	19.103	2685	2689	2695	rBV2	277638	607822	7.60%	0.819%
45	19.245	2709	2713	2718	rBV3	147384	294694	3.68%	0.397%
46	19.368	2729	2734	2739	rBV	2813666	3684287	46.07%	4.964%
47	19.421	2740	2743	2747	rBV4	158534	197416	2.47%	0.266%
48	19.480	2750	2753	2757	rVV2	237253	309016	3.86%	0.416%
49	19.703	2786	2791	2792	rBV2	481824	672955	8.41%	0.907%
50	19.727	2792	2795	2804	rVB	2422914	3508984	43.88%	4.728%
51	19.933	2825	2830	2834	rBV	6770088	7997510	100.00%	10.776%
52	20.321	2894	2896	2900	rVB	312011	341534	4.27%	0.460%
53	21.197	3042	3045	3053	rVB3	801873	1197464	14.97%	1.613%
54	21.492	3089	3095	3099	rBV2	2768552	5058251	63.25%	6.815%
55	21.533	3099	3102	3112	rVB	1036637	1518063	18.98%	2.045%
56	23.909	3502	3506	3511	rVB2	1489718	2554214	31.94%	3.441%

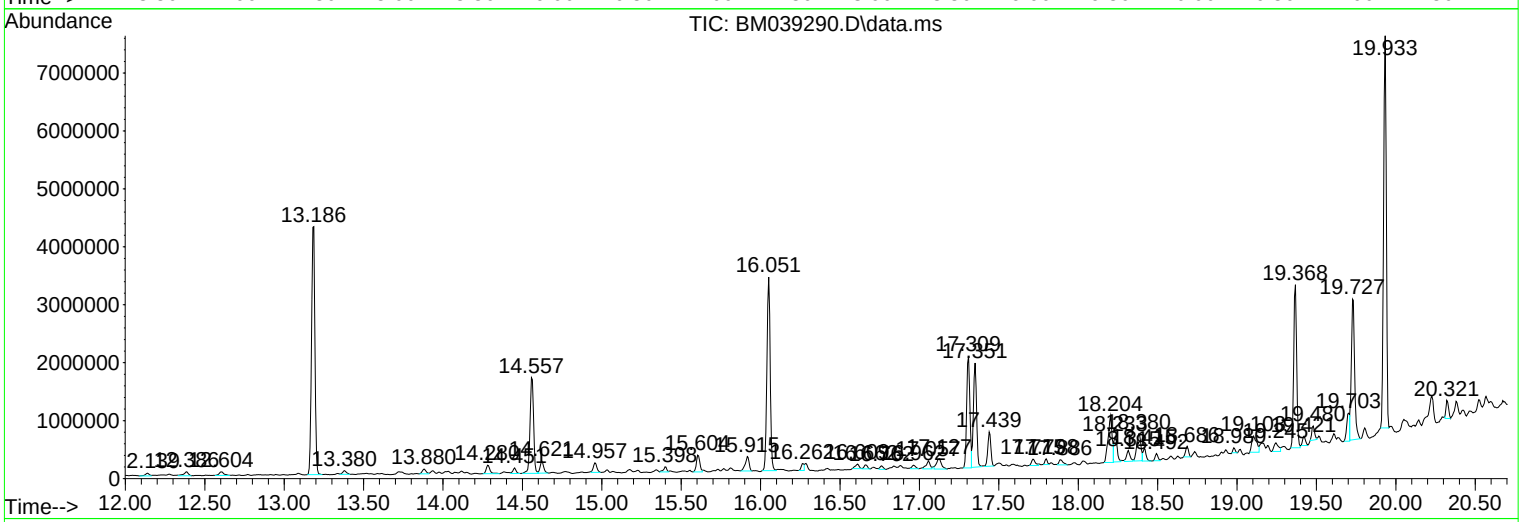
Sum of corrected areas: 74218146

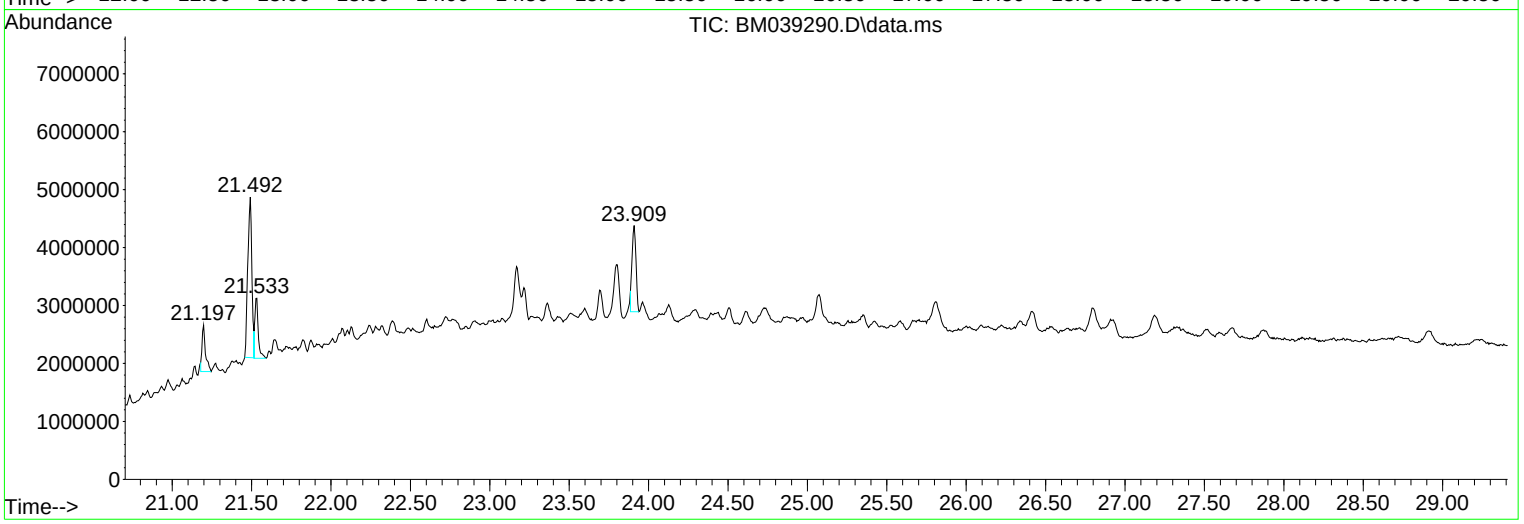
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
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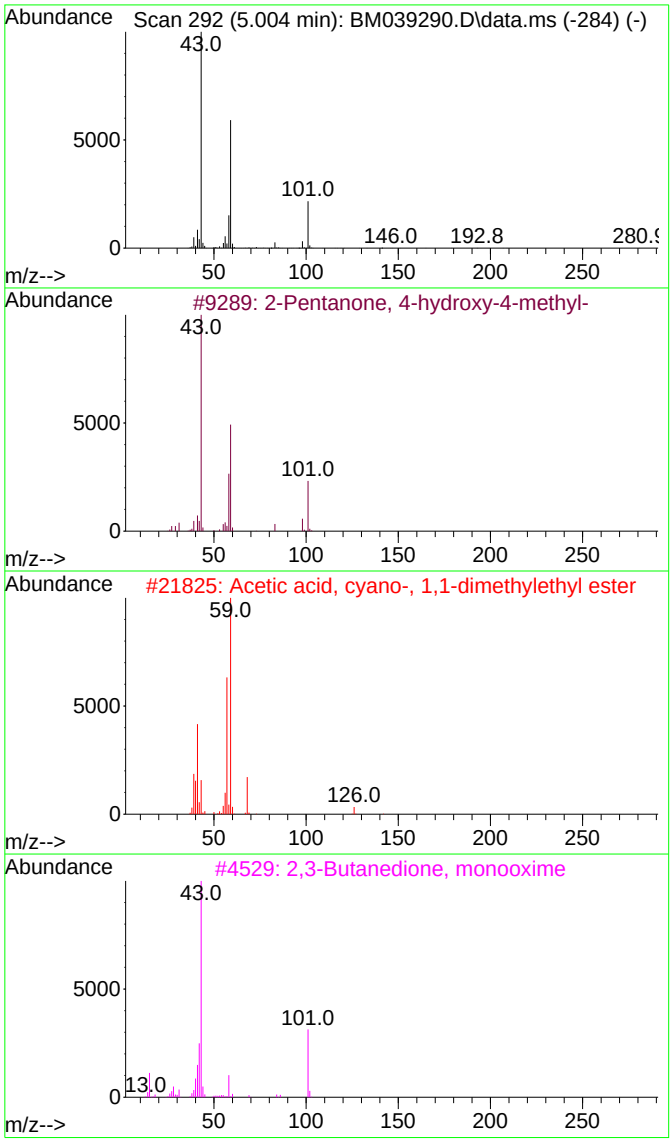
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

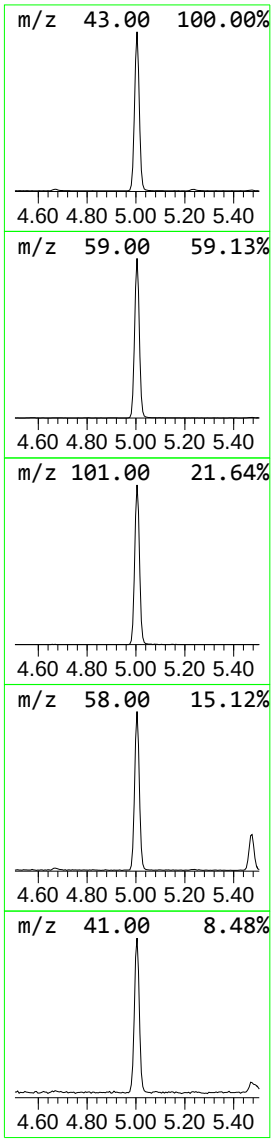
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	27.21 ng	1986910	1,4-Dichlorobenzene-d4	7.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

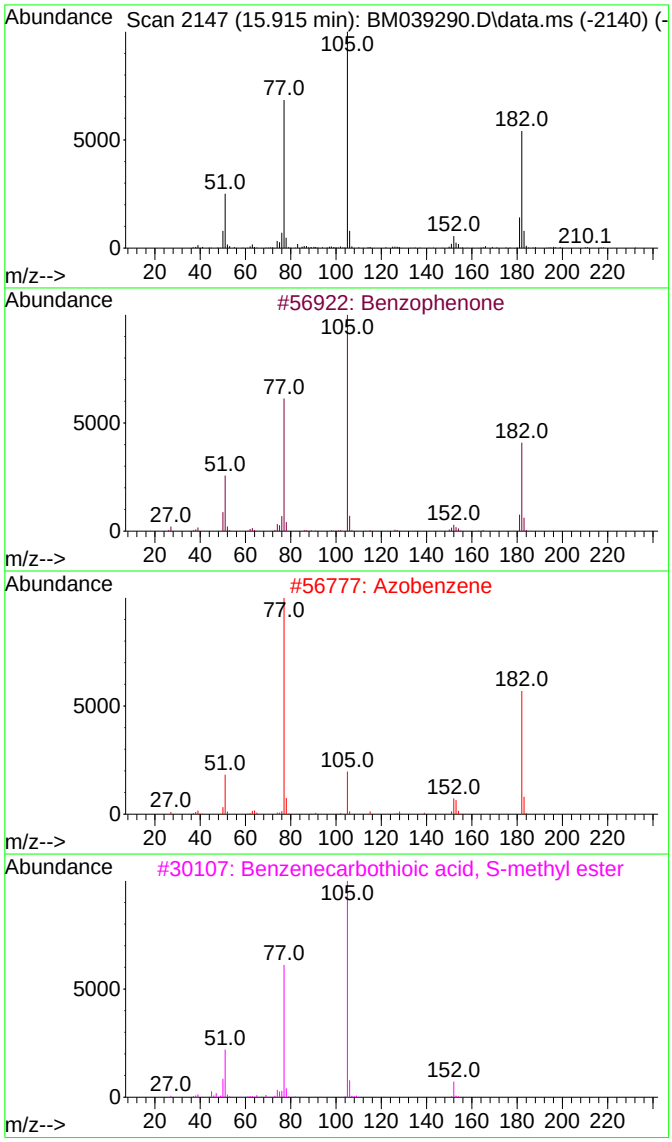
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

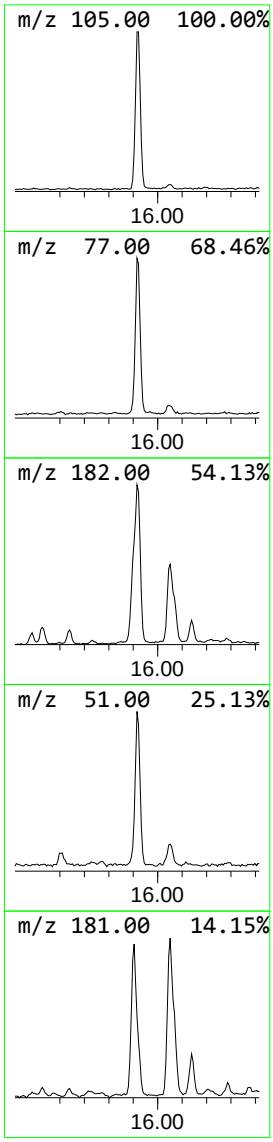
****

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	3.33 ng	420287	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	58
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

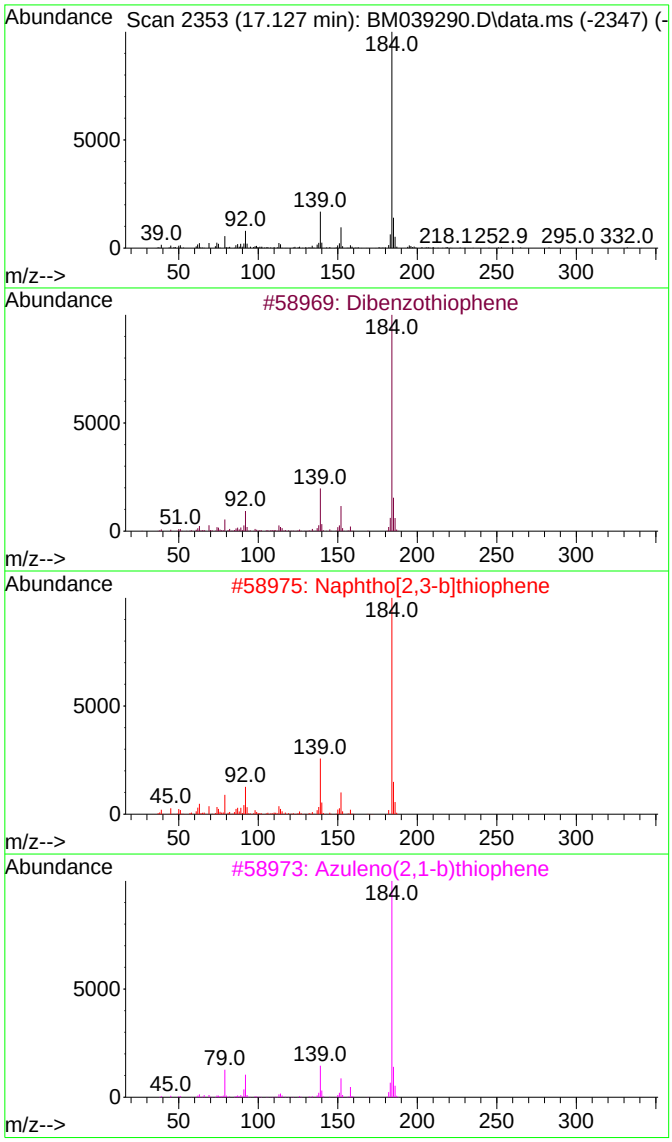
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

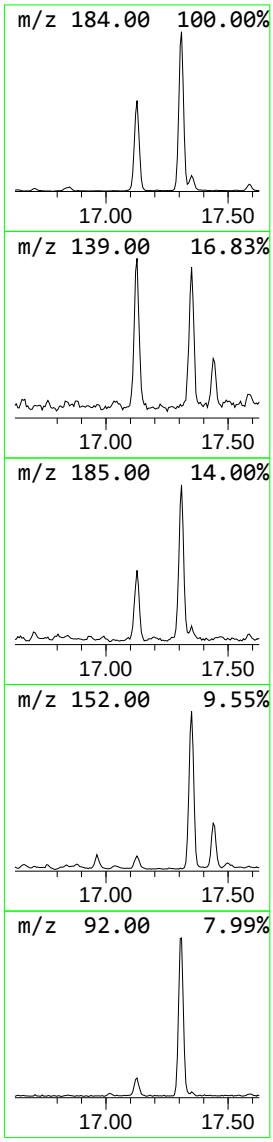
****

Peak Number 3 Dibenzothiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.127	2.82 ng	383260	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	95
2	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	90
3	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	90
4	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	80
5	Thianthrene, 5-oxide	232	C12H8OS2	002362-50-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

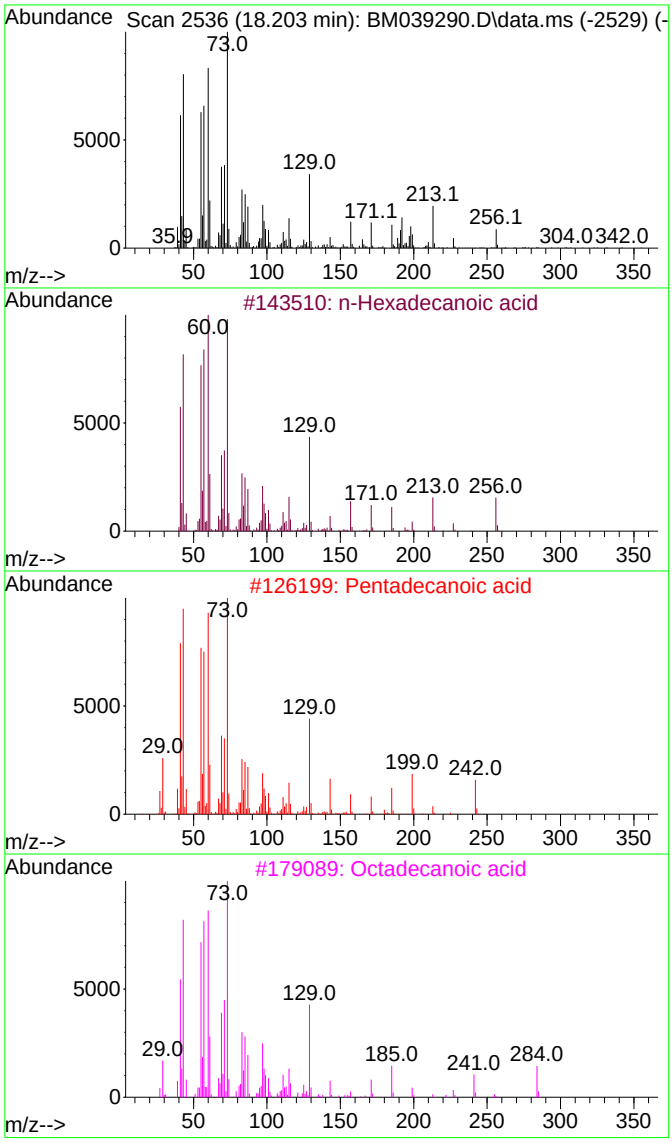
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

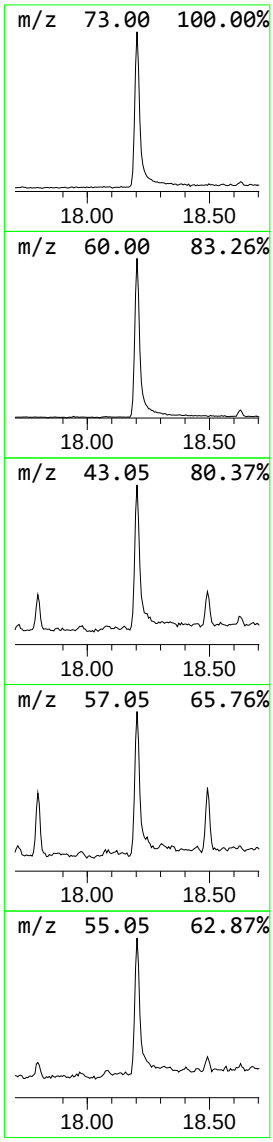
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.203	10.69 ng	1452950	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

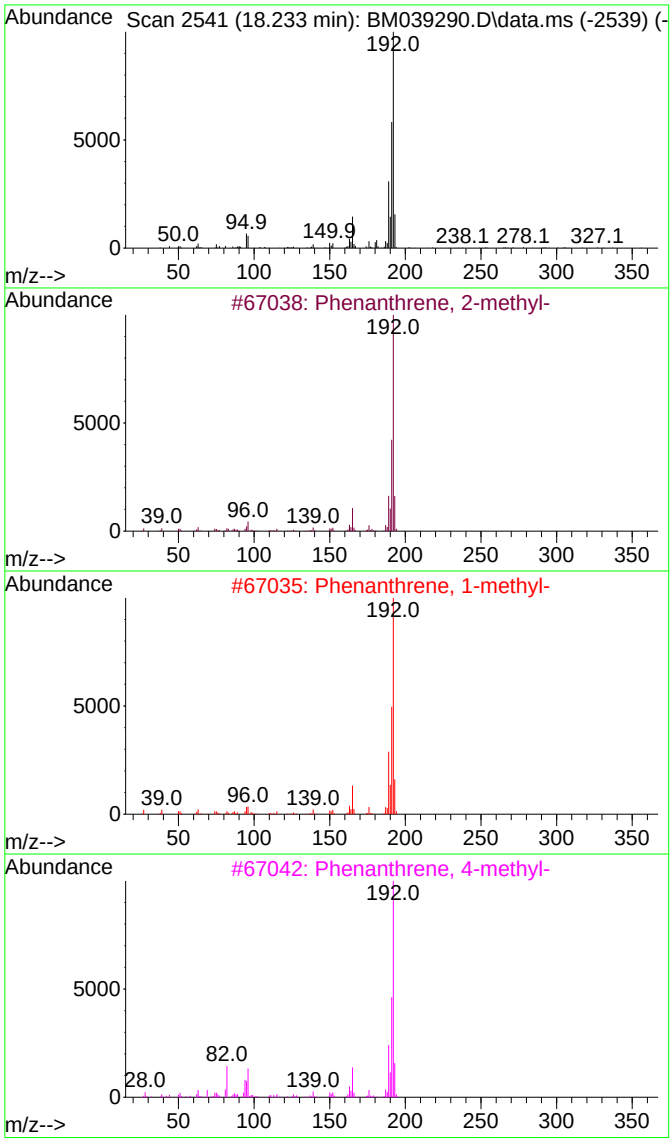
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

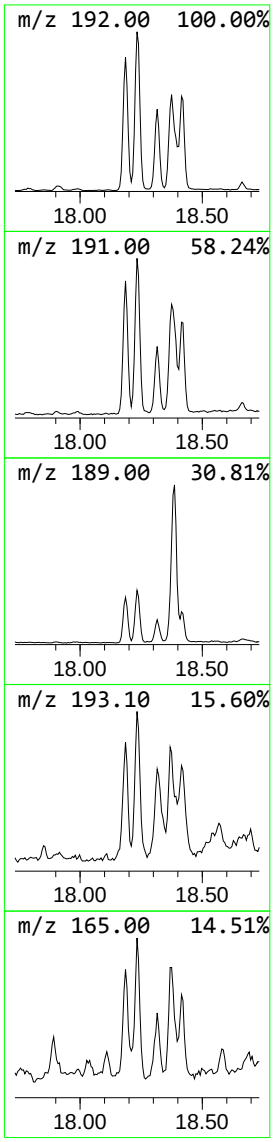
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	4.40 ng	598057	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

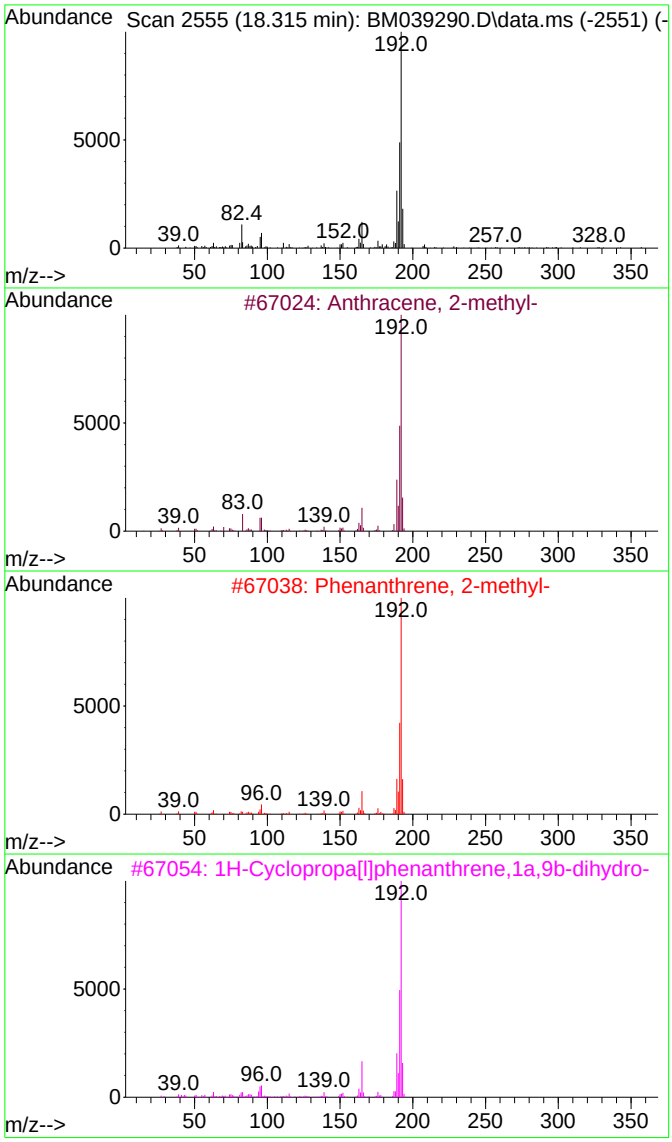
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

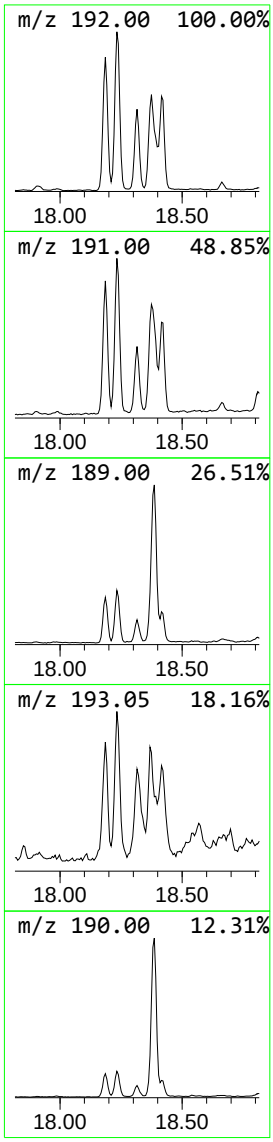
****

Peak Number 6 Anthracene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.315	2.12 ng	287523	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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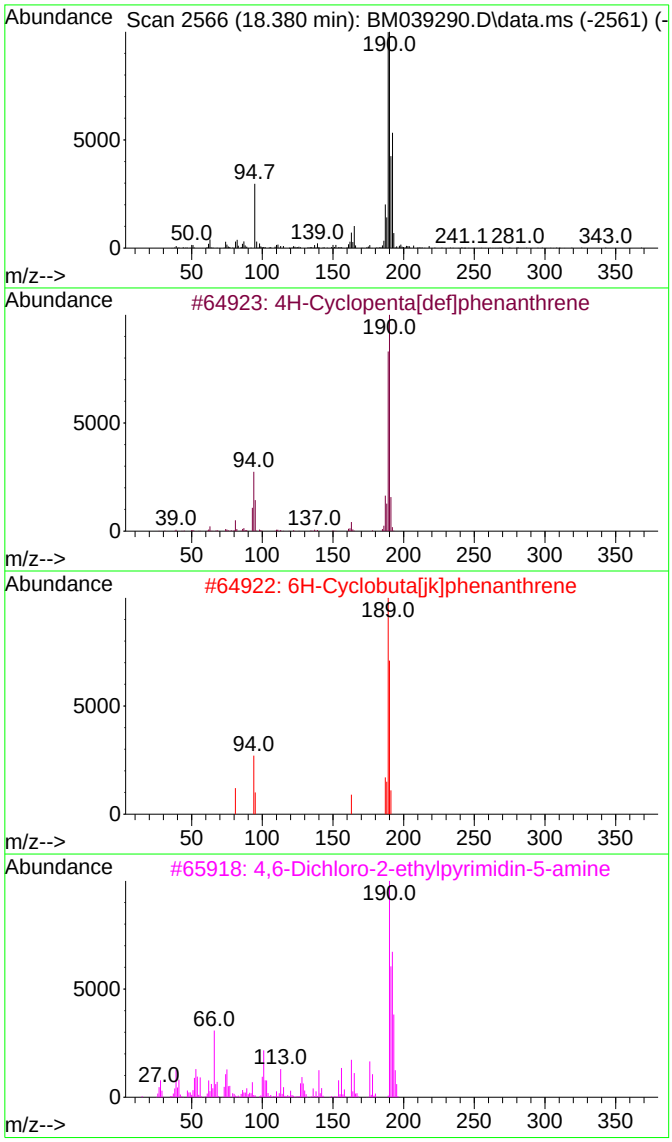
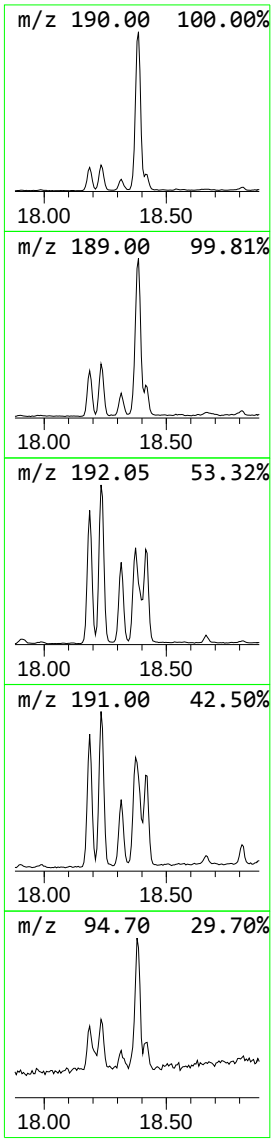
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.380	6.44 ng	875382	Phenanthrene-d10	17.309

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	50
3	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	43
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

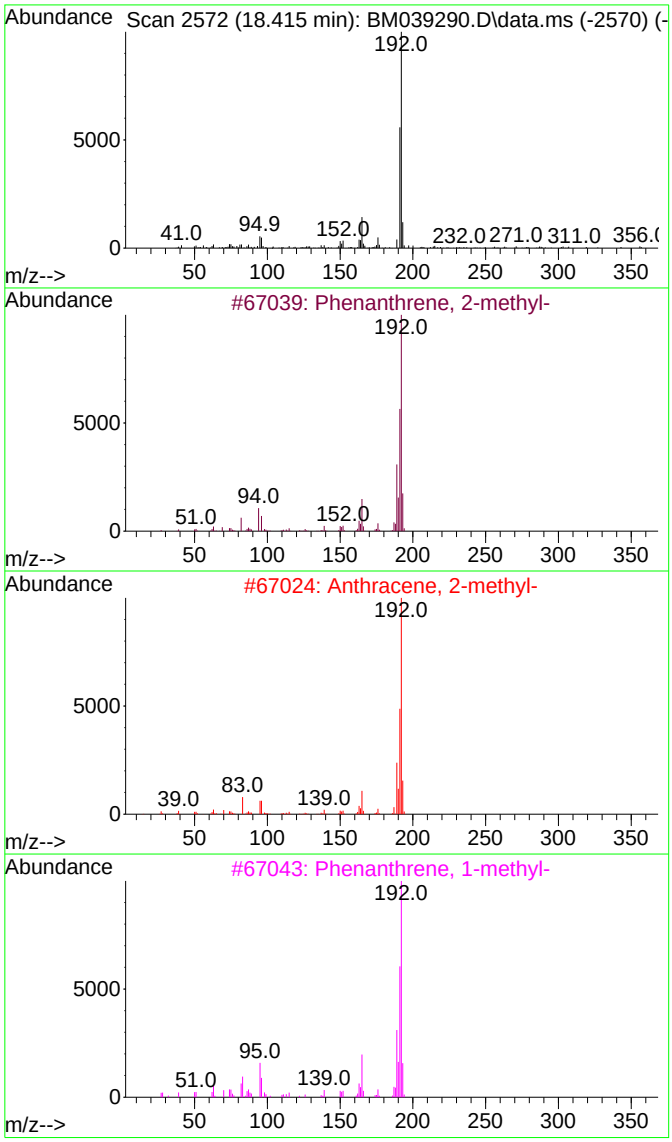
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

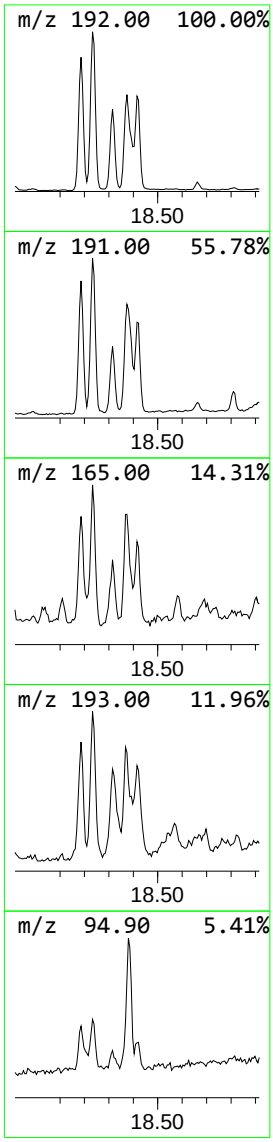
****

Peak Number 8 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.415	2.06 ng	280232	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

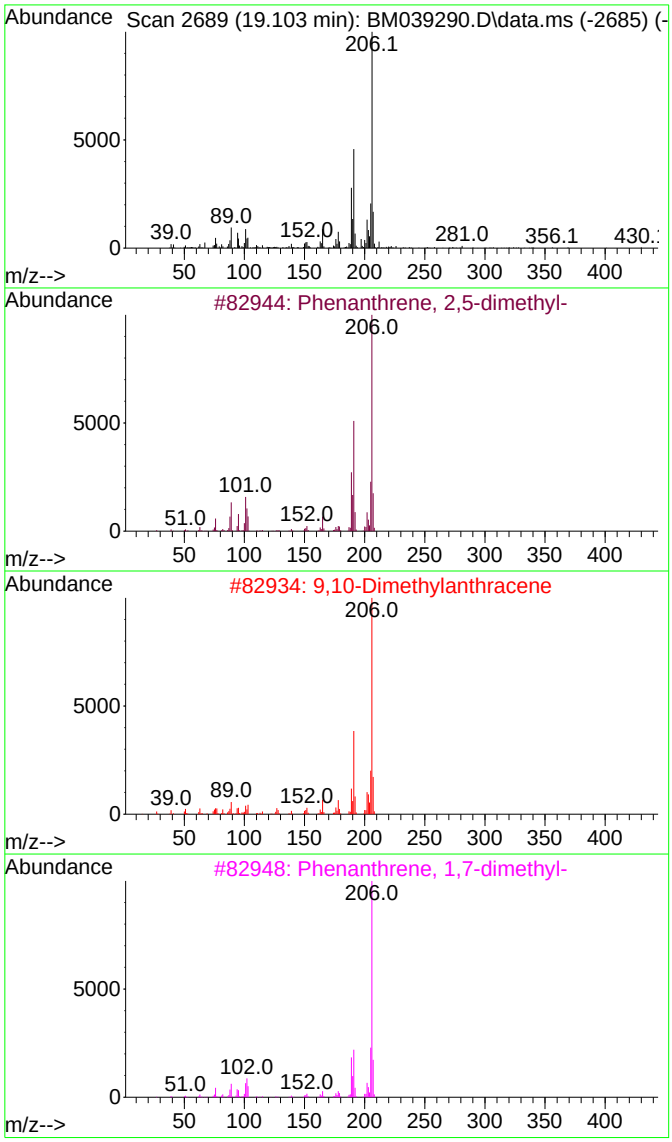
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

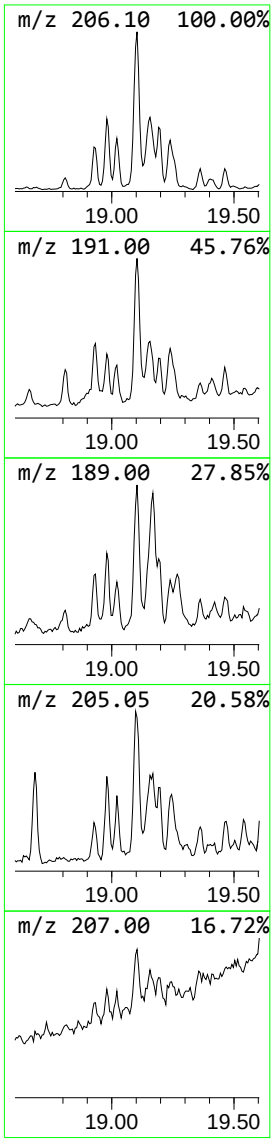
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.104	4.47 ng	607822	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	96
3	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
5	di-p-Tolylacetylene	206	C16H14	002789-88-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

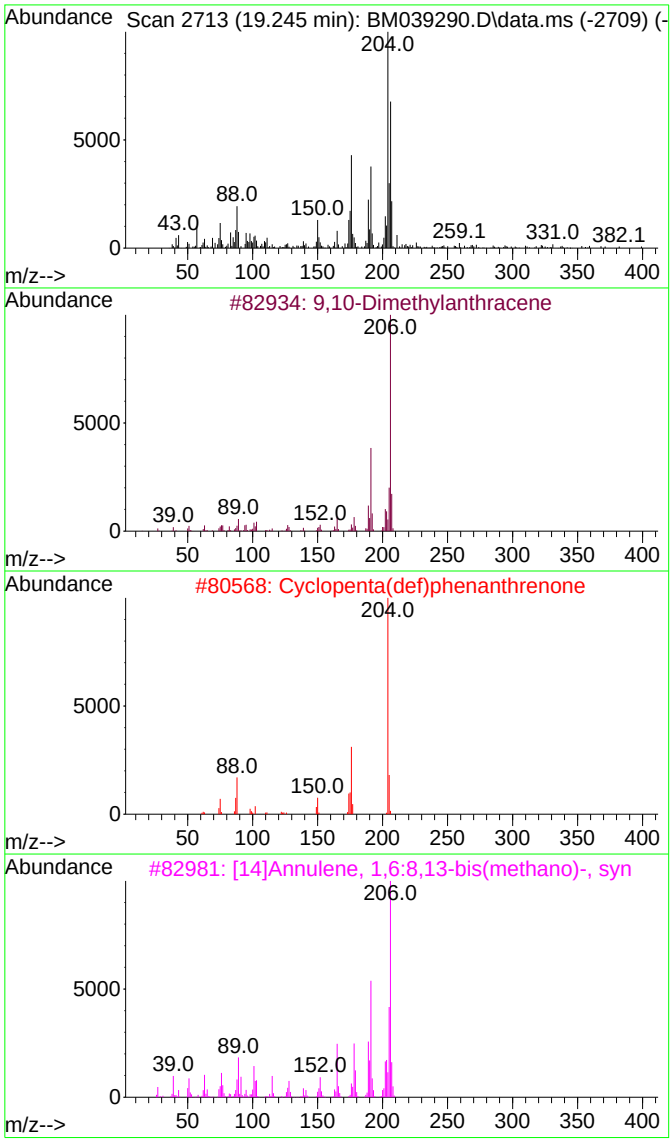
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

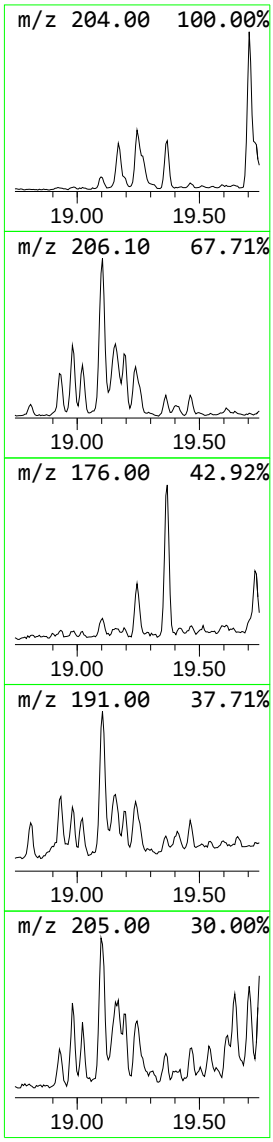
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 9,10-Dimethylanthracene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	2.17 ng	294694	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	70
2	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	55
3	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	38
4	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	38
5	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

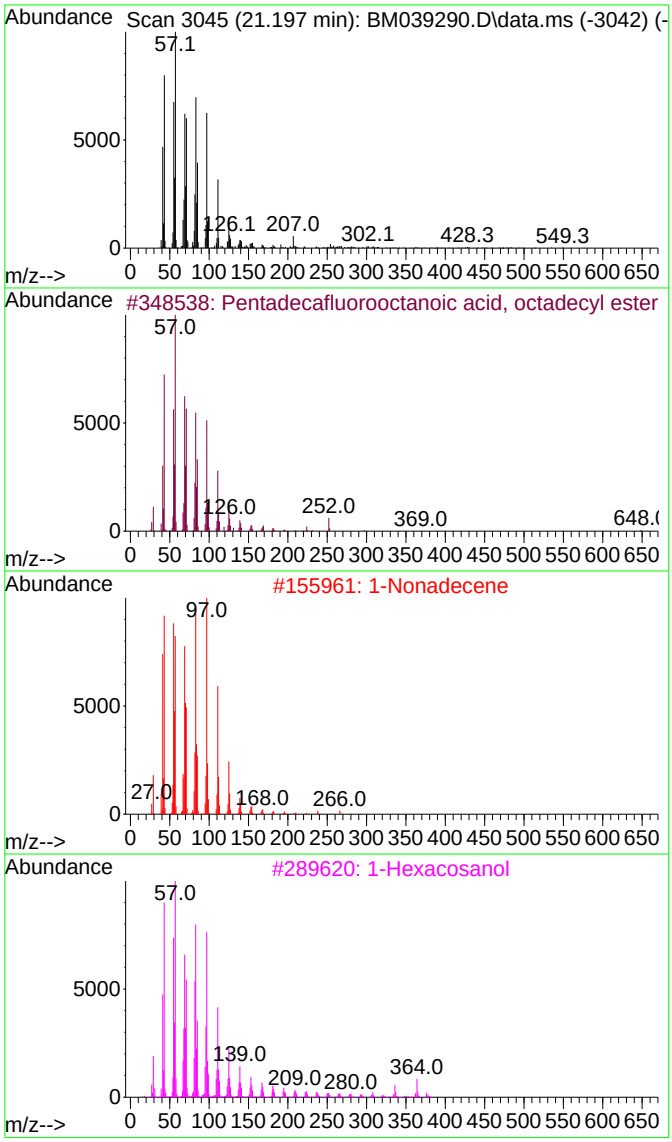
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

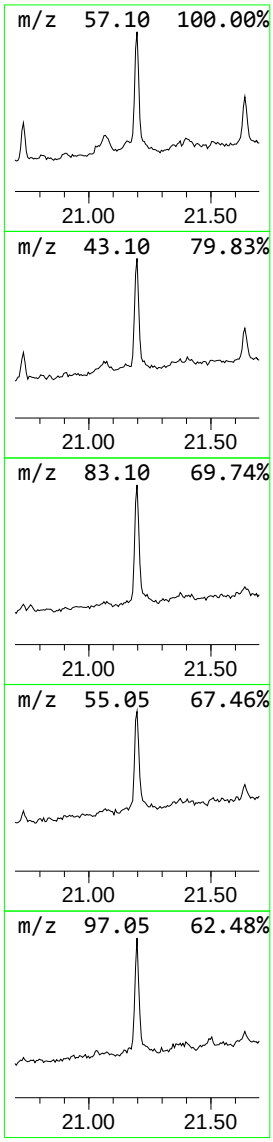
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.197	4.73 ng	1197460	Chrysene-d12	21.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	1-Nonadecene	266	C19H38	018435-45-5	93
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039290.D
Acq On : 03 Apr 2023 21:55
Operator : CG/JU
Sample : 02162-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	27.2	ng	1986910	1	7.916	1460560	20.0
Benzophenone	15.915	3.3	ng	420287	3	14.557	2527120	20.0
Dibenzothiophene	17.127	2.8	ng	383260	4	17.309	2718480	20.0
n-Hexadecanoic ...	18.203	10.7	ng	1452950	4	17.309	2718480	20.0
Phenanthrene, 2...	18.233	4.4	ng	598057	4	17.309	2718480	20.0
Anthracene, 2-m...	18.315	2.1	ng	287523	4	17.309	2718480	20.0
4H-Cyclopenta[d...	18.380	6.4	ng	875382	4	17.309	2718480	20.0
Phenanthrene, 1...	18.415	2.1	ng	280232	4	17.309	2718480	20.0
Phenanthrene, 2...	19.104	4.5	ng	607822	4	17.309	2718480	20.0
9,10-Dimethylan...	19.245	2.2	ng	294694	4	17.309	2718480	20.0
Pentadecafluoro...	21.197	4.7	ng	1197460	5	21.491	5058250	20.0