LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CL-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_G\Methods\8270-BG082222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054712.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.789	80	85	93	rBV	27248	43591	1.57%	0.258%
2	5.228	323	330	339	rVB	79667	131528	4.73%	0.778%
3	5.698	403	410	420	rBV	833534	1346963	48.47%	7.971%
4	7.302	673	683	693	rBV	845539	1448412	52.12%	8.571%
5	8.160	822	829	836	rBV	195320	337987	12.16%	2.000%
6	9.030	969	977	986	rBV	58860	104708	3.77%	0.620%
7	9.329	1020	1028	1035	rBV	489696	892379	32.11%	5.281%
8	10.986	1302	1310	1317	rBV	276610	502035	18.06%	2.971%
9	13.419	1715	1724	1733	rVB	1319183	2127065	76.53%	12.587%
10	14.788	1946	1957	1964	rBV	425202	675971	24.32%	4.000%
11	16.274	2201	2210	2218	rBV	936934	1461064	52.57%	8.646%
12	17.532	2418	2424	2429	rBV	463028	753059	27.10%	4.456%
13	17.573	2429	2431	2437	rVB	111001	155497	5.59%	0.920%
14	18.113	2518	2523	2529	rVB	26619	41847	1.51%	0.248%
15	18.337	2555	2561	2567	rBV4	13374	28609	1.03%	0.169%
16	18.407	2567	2573	2578	rVV2	120419	215805	7.76%	1.277%
17	18.454	2578	2581	2589	rVB	78375	123183	4.43%	0.729%
18	18.595	2600	2605	2609	rBV3	58841	105368	3.79%	0.624%
19	18.636	2609	2612	2619	rVB	52858	78453	2.82%	0.464%
20	18.901	2652	2657	2660	rBV3	31464	46161	1.66%	0.273%
21	18.942	2660	2664	2675	rVB3	24537	52756	1.90%	0.312%
22	19.194	2703	2707	2711	rBV	25784	32402	1.17%	0.192%
23	19.318	2722	2728	2732	rBV	72520	119455	4.30%	0.707%
24	19.365	2732	2736	2740	rBV3	26238	47189	1.70%	0.279%
25	19.406	2740	2743	2747	rVB	22017	28447	1.02%	0.168%
26	19.453	2747	2751	2758	rBV4	30222	64677	2.33%	0.383%
27	19.576	2767	2772	2778	rVB	107385	162580	5.85%	0.962%
28	19.670	2785	2788	2795	rVB3	36236	53623	1.93%	0.317%
29	19.941	2829	2834	2841	rVB	179976	274537	9.88%	1.625%
30	20.011	2841	2846	2851	rVB2	27737	42333	1.52%	0.251%
31	20.134	2861	2867	2881	rVB	2101873	2779214	100.00%	16.447%
32	20.264	2883	2889	2897	rBV5	27843	79633	2.87%	0.471%
33	20.399	2907	2912	2914	rBV4	27987	48465	1.74%	0.287%
34	20.428	2914	2917	2925	rVB2	40367	59730	2.15%	0.353%
35	20.587	2940	2944	2948	rBV	43490	58246	2.10%	0.345%
36	20.728	2964	2968	2972	rBV	45501	62503	2.25%	0.370%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-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_G\Methods\8270-BG082222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.775	2972	2976	2980	rVV	31316	43572	1.57%	0.258%
38	21.198	3044	3048	3055	rVB	30502	60246	2.17%	0.357%
39	21.445	3085	3090	3096	rBV	117454	176508	6.35%	1.045%
40	21.697	3131	3133	3140	rVB	29004	39818	1.43%	0.236%
41	21.827	3147	3155	3161	rBV	464848	874244	31.46%	5.174%
42	21.874	3161	3163	3172	rVB	56204	94388	3.40%	0.559%
43	22.661	3292	3297	3309	rBV7	33701	97071	3.49%	0.574%
44	23.754	3480	3483	3488	rVB5	28464	48110	1.73%	0.285%
45	25.205	3720	3730	3745	rVB2	249459	774001	27.85%	4.580%
46	26.456	3936	3943	3953	rVB3	34067	104926	3.78%	0.621%

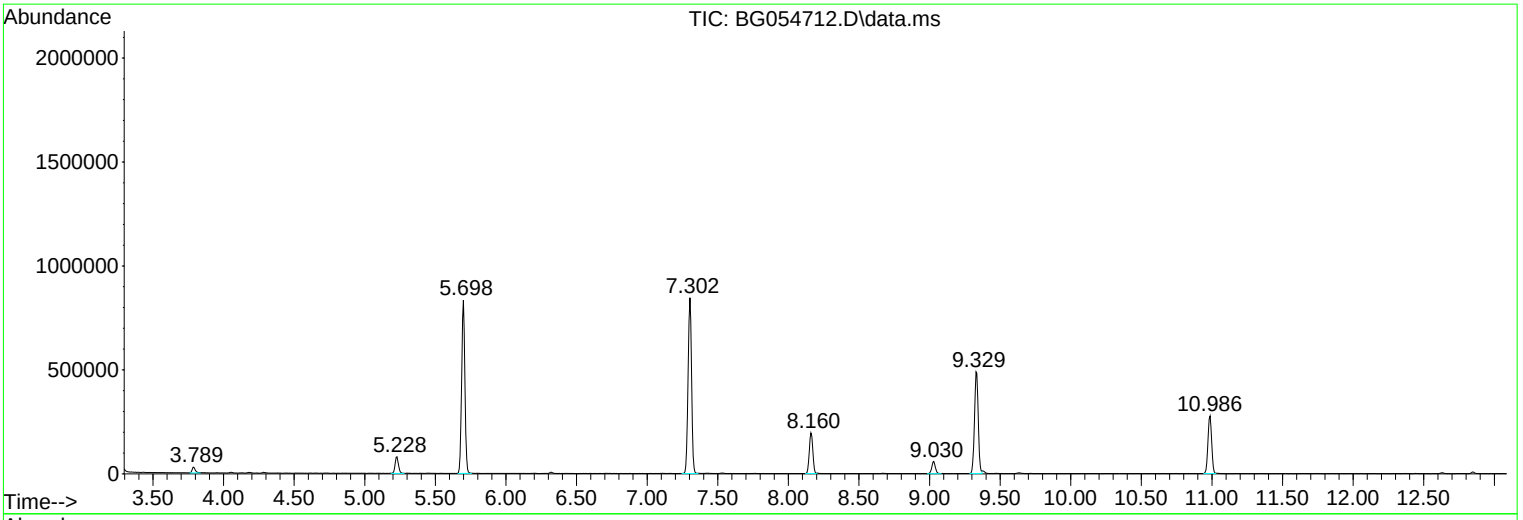
Sum of corrected areas: 16898359

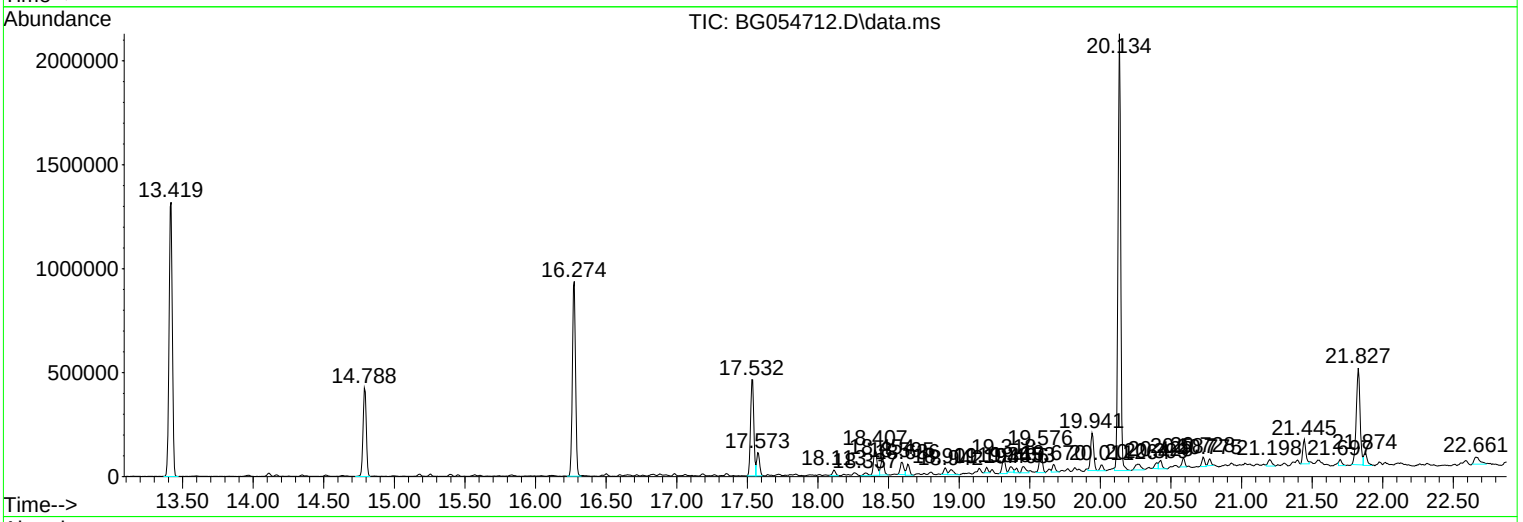
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

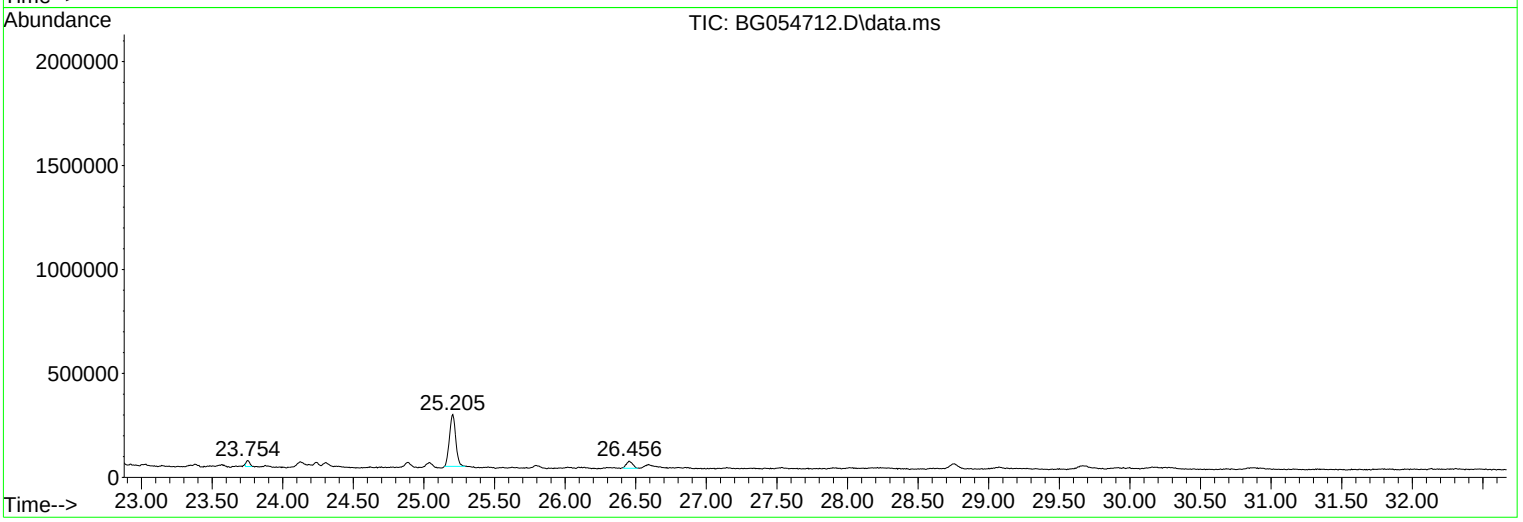
Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.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_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

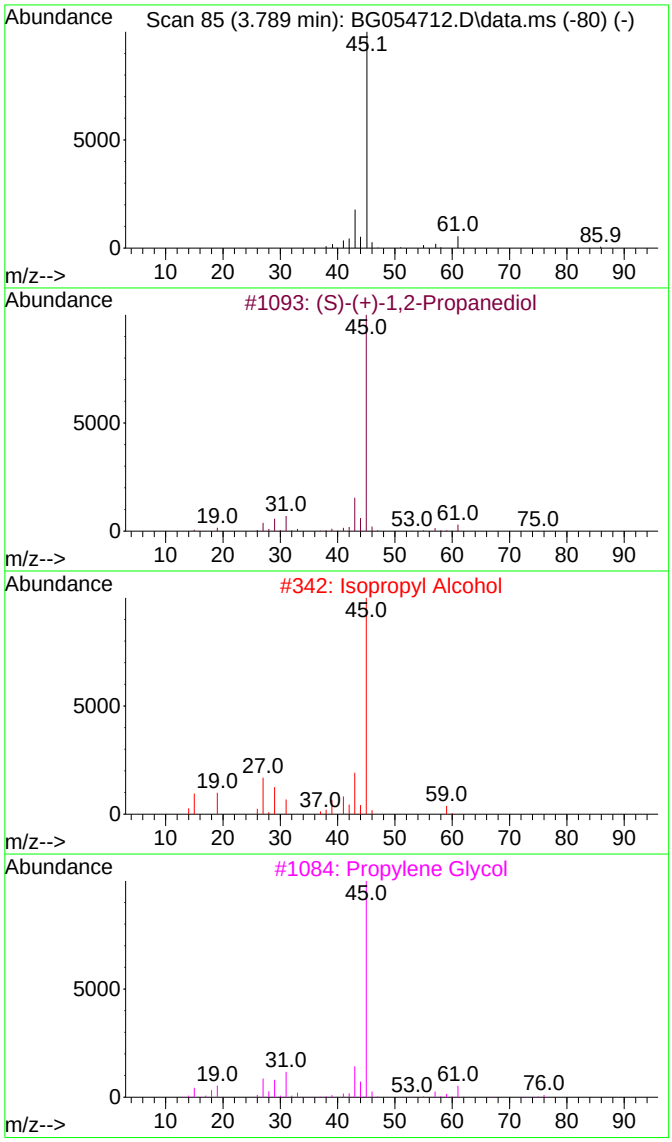
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

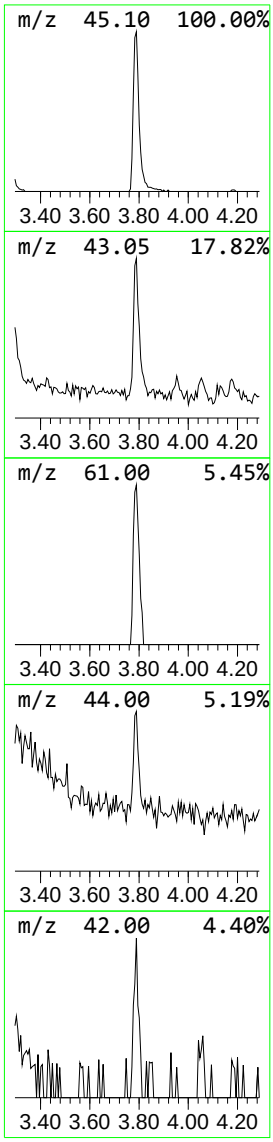
****

Peak Number 1 unknown3.789 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	2.58 ng	43591	1,4-Dichlorobenzene-d4	8.160

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	Formamide	45	CH3NO	000075-12-7	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

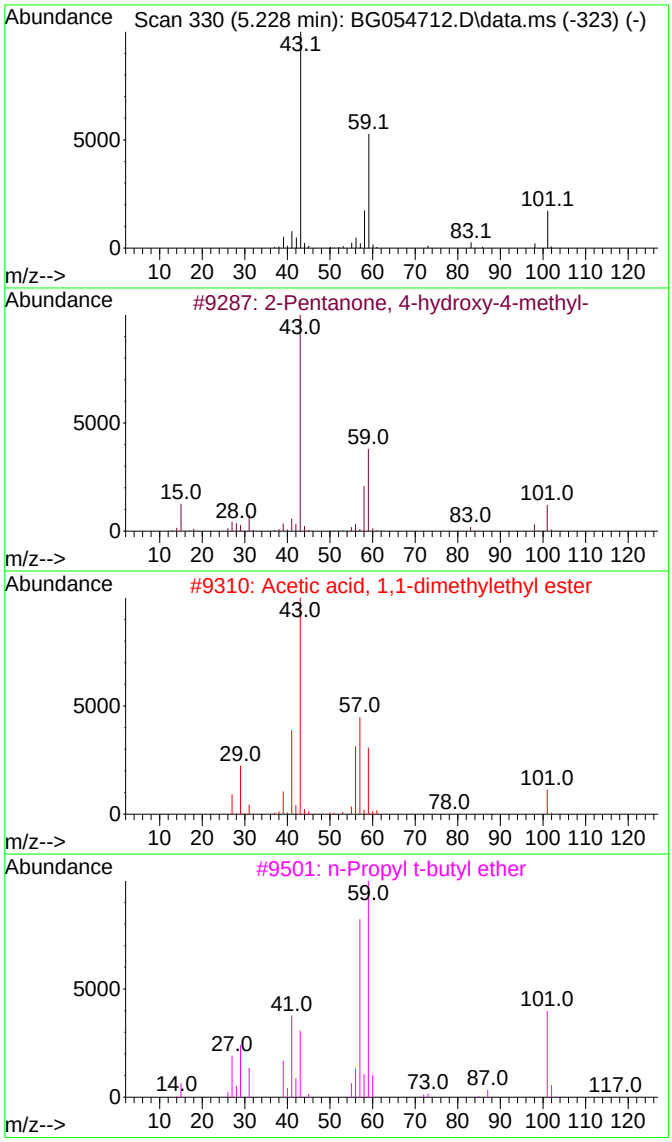
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

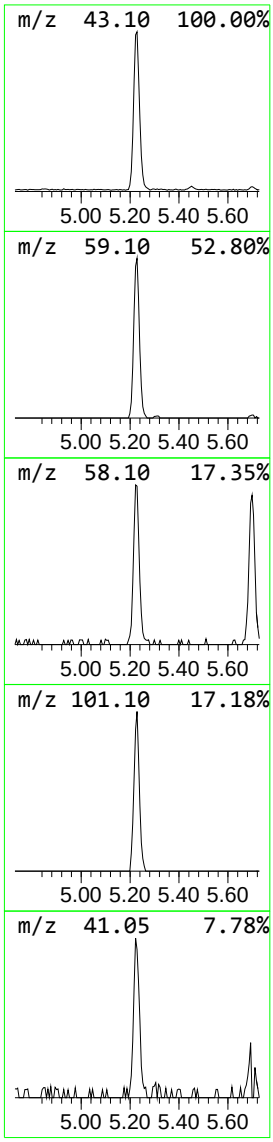
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.228	7.78 ng	131528	1,4-Dichlorobenzene-d4	8.160

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

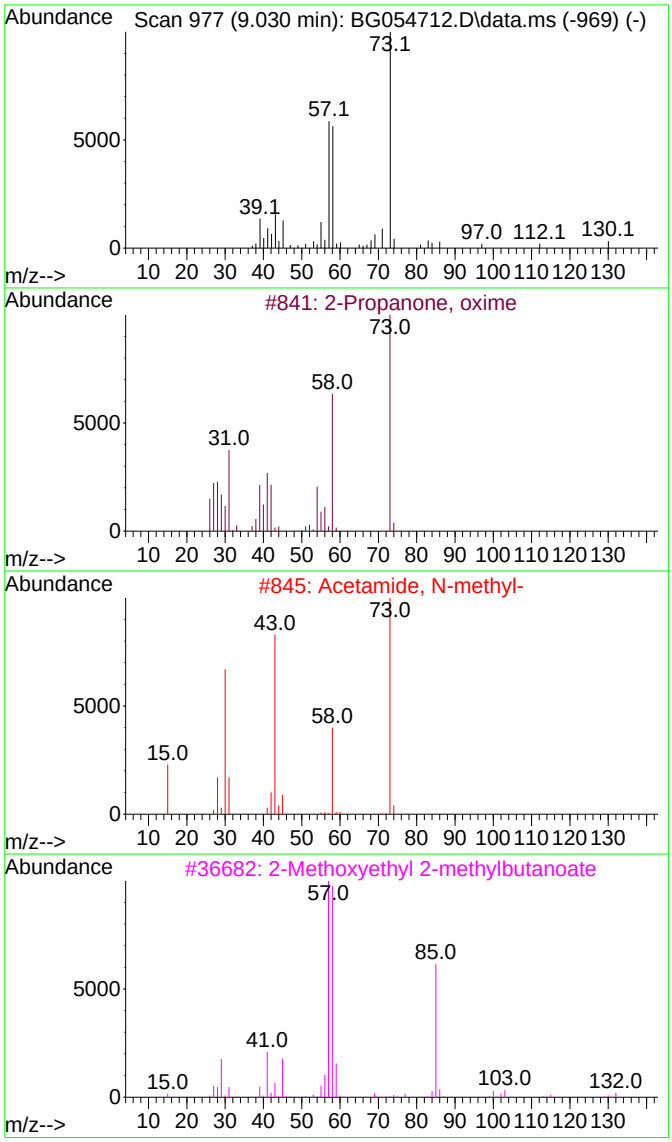
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

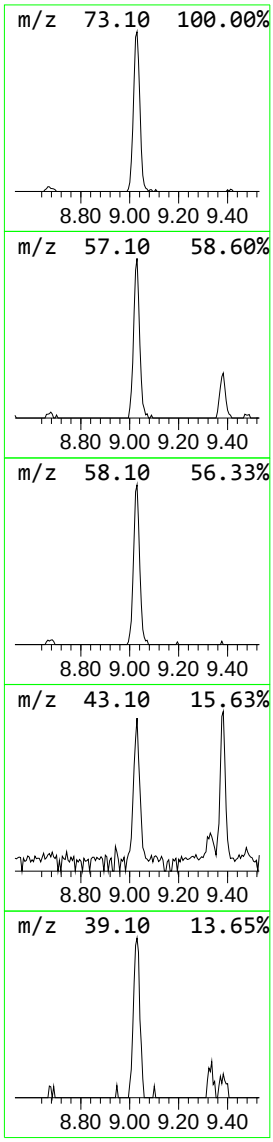
****

Peak Number 3 unknown9.030 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.030	6.20 ng	104708	1,4-Dichlorobenzene-d4	8.160

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, oxime	73	C3H7NO	000127-06-0	47
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	42
3	2-Methoxyethyl 2-methylbutanoate	160	C8H16O3	1000366-96-4	33
4	Glycinamide, N,N,N(2),N(2)-tetra...	130	C6H14N2O	1000452-64-2	32
5	Acetic acid, 2-(dimethylamino)et...	131	C6H13NO2	001421-89-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

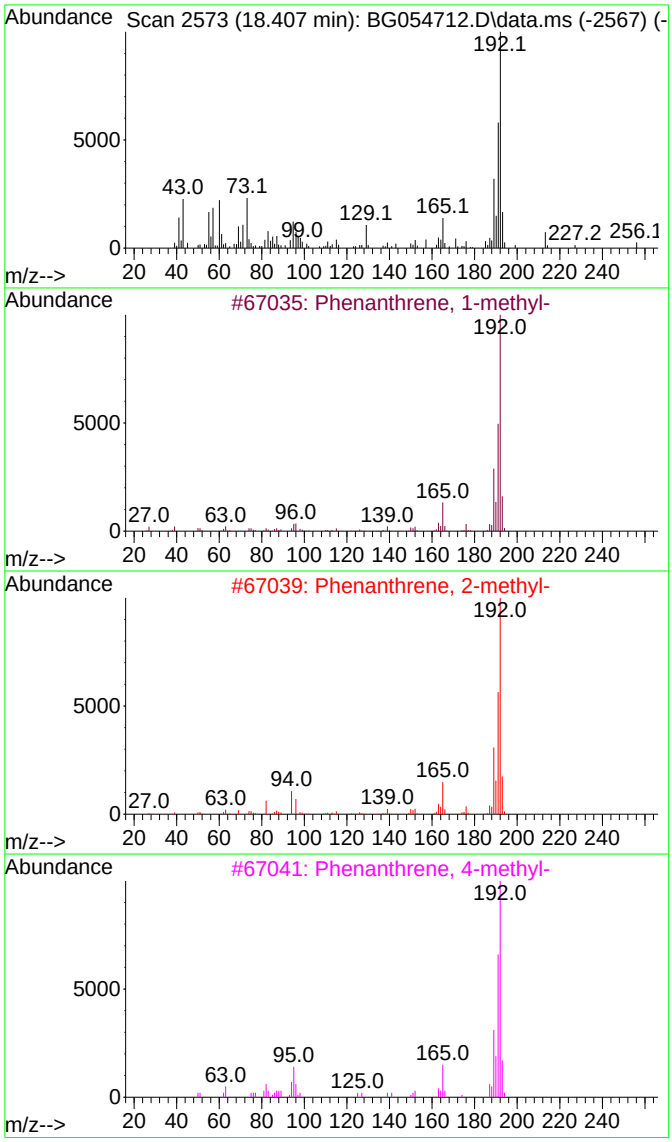
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

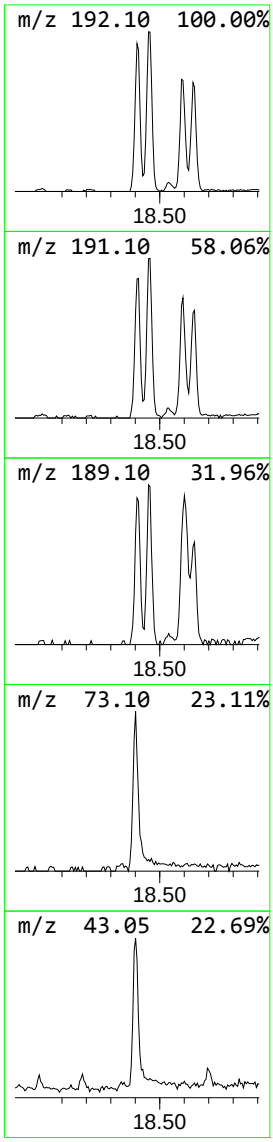
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.407	5.73 ng	215805	Phenanthrene-d10	17.538

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	96
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

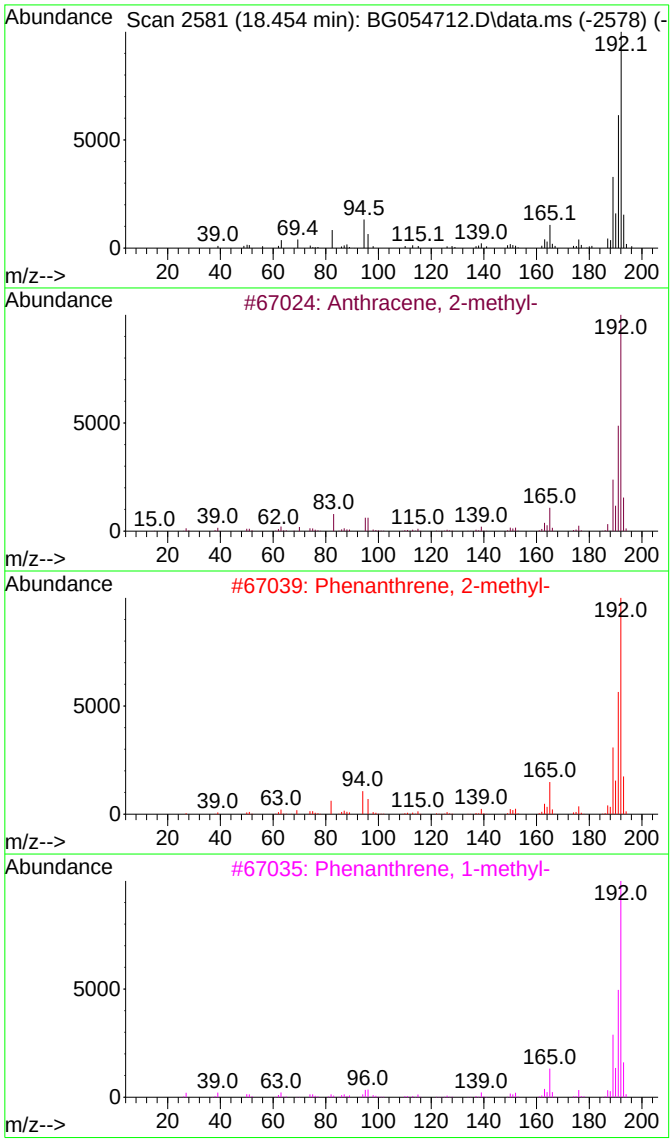
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

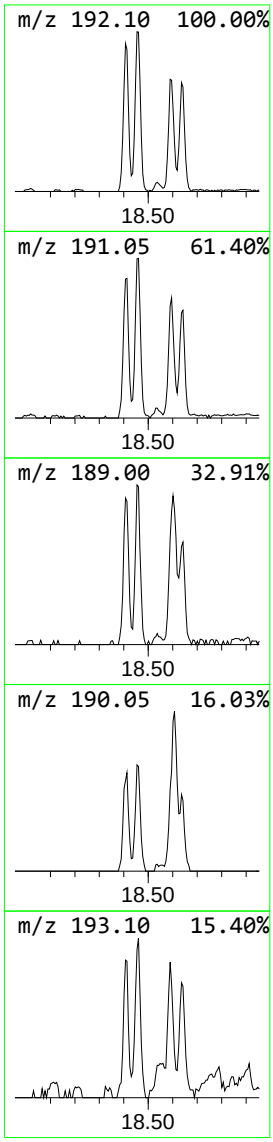
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.454	3.27 ng	123183	Phenanthrene-d10	17.538

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

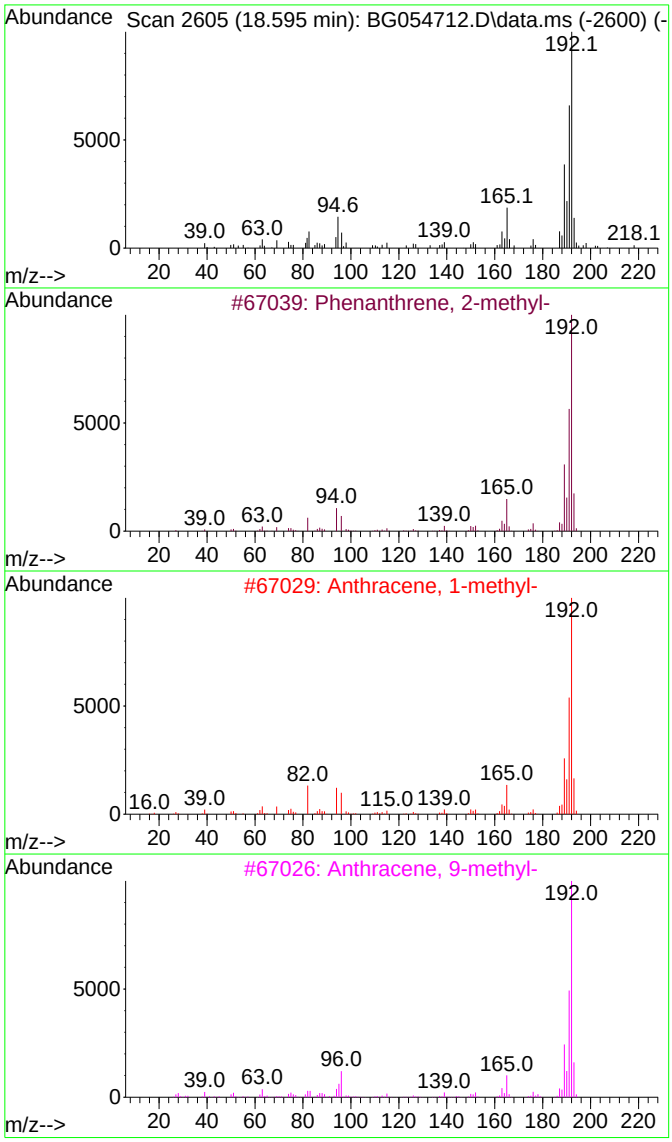
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

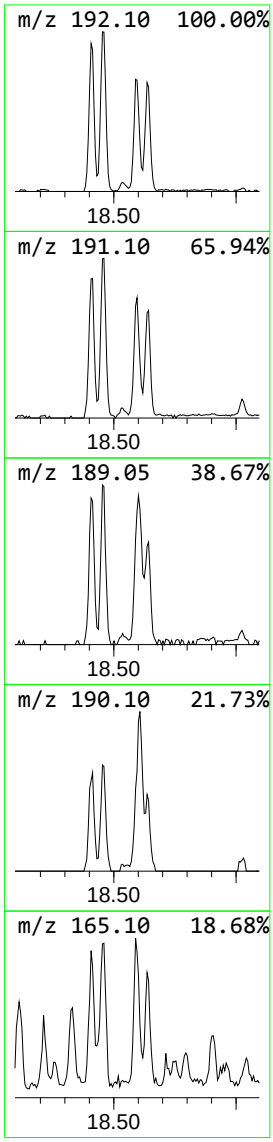
****

Peak Number 6 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.595	2.80 ng	105368	Phenanthrene-d10	17.538

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	83
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

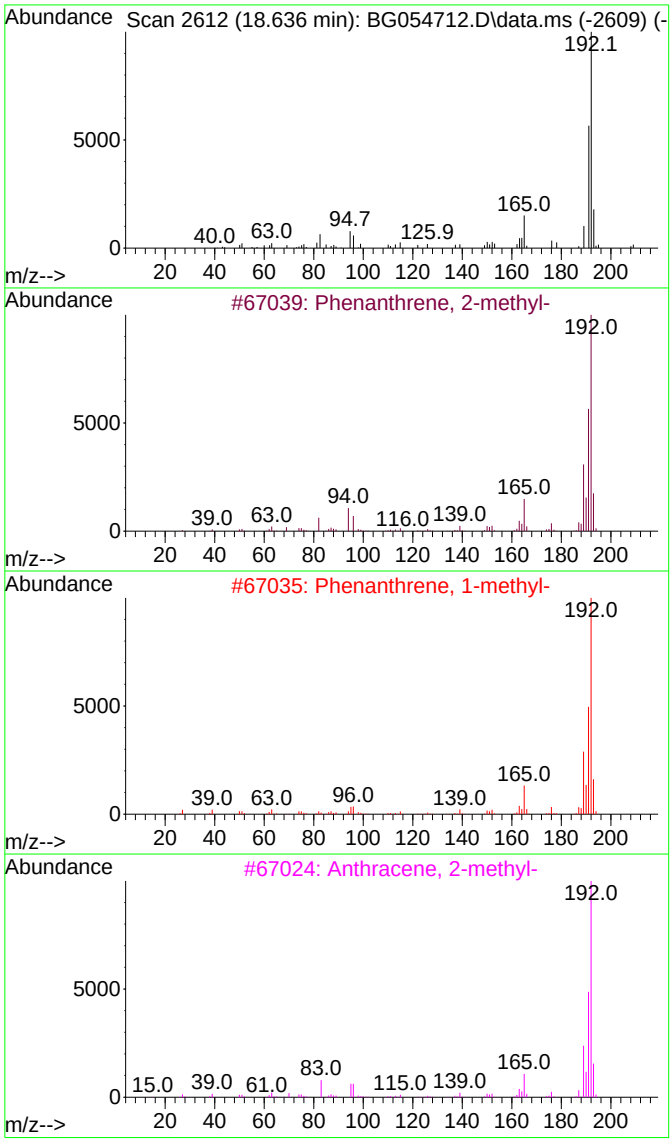
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

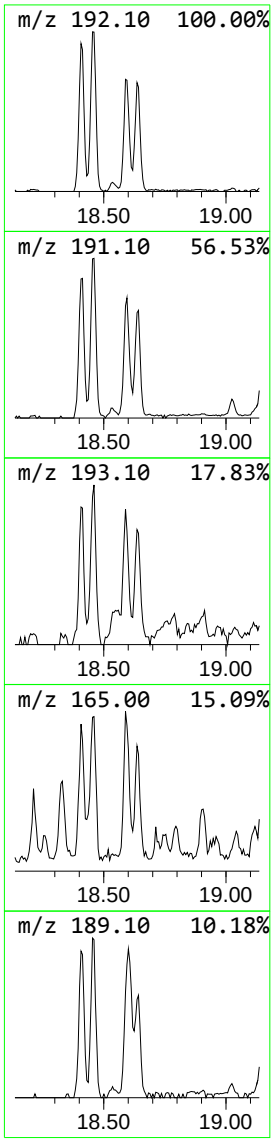
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Cyclopropa[l]phenanthren... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.636	2.08 ng	78453	Phenanthrene-d10	17.538

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

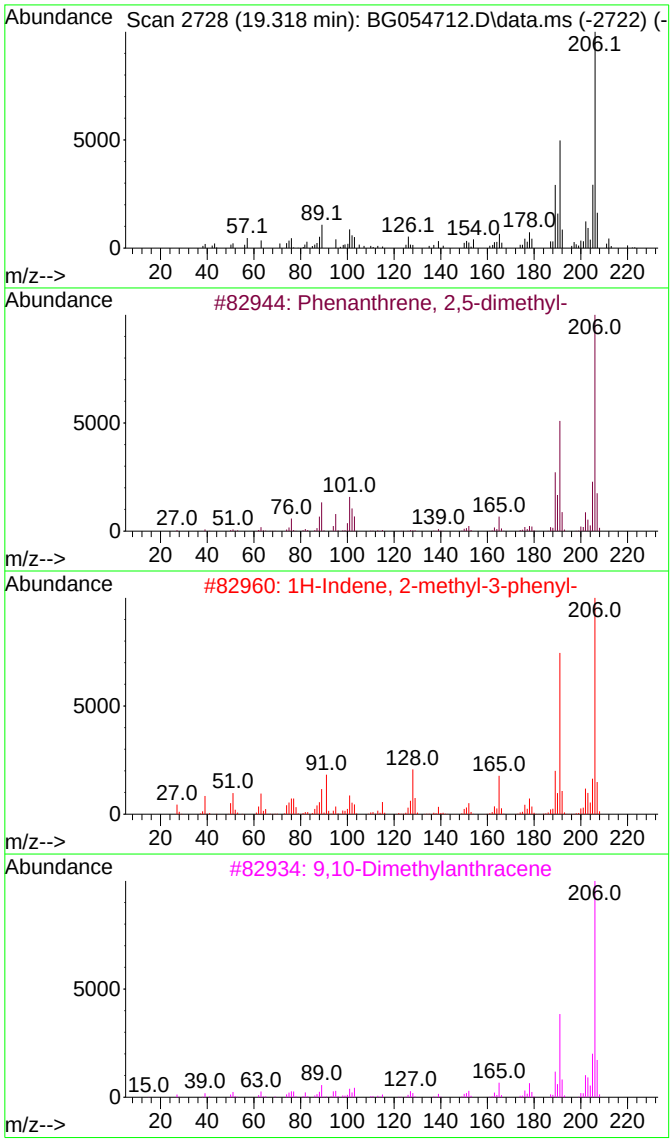
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

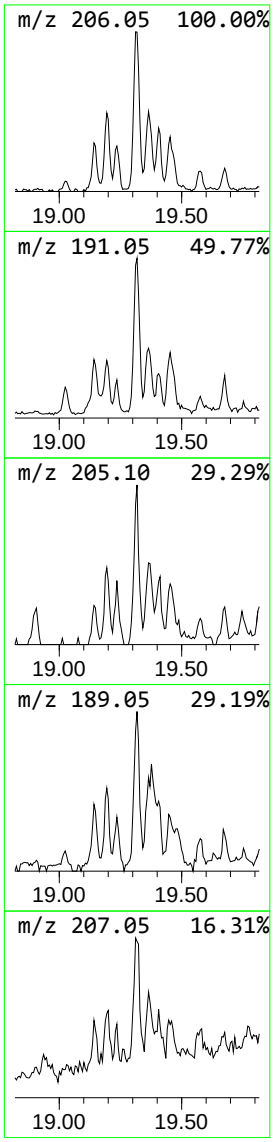
****

Peak Number 8 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.318	3.17 ng	119455	Phenanthrene-d10	17.538

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
2	1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	90
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	87
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	87
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

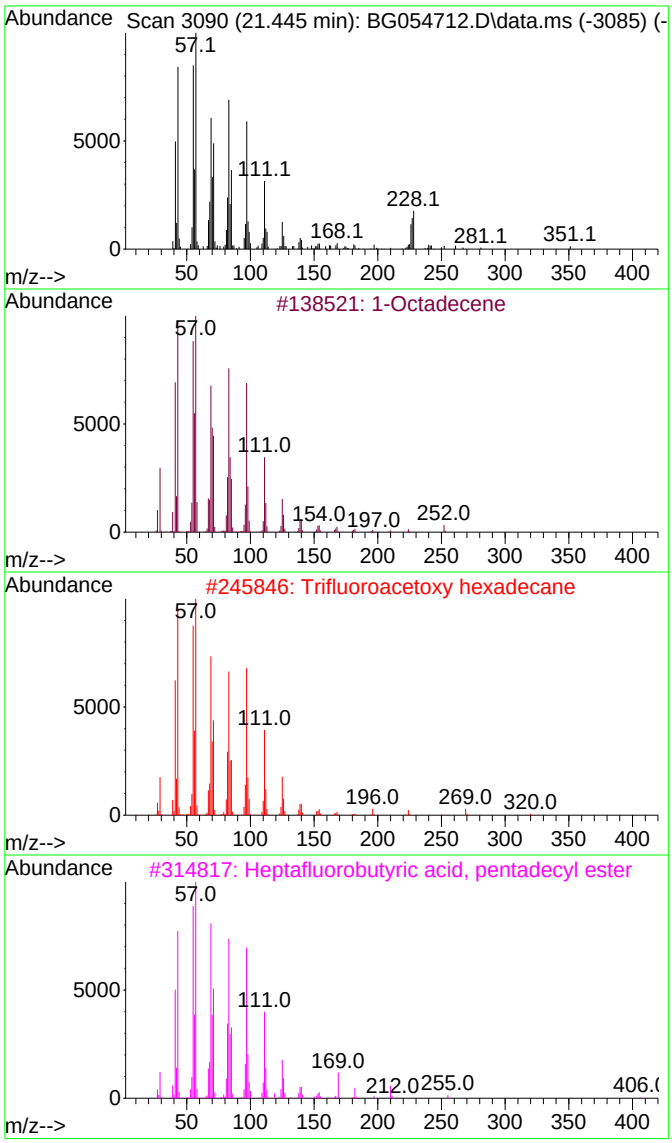
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

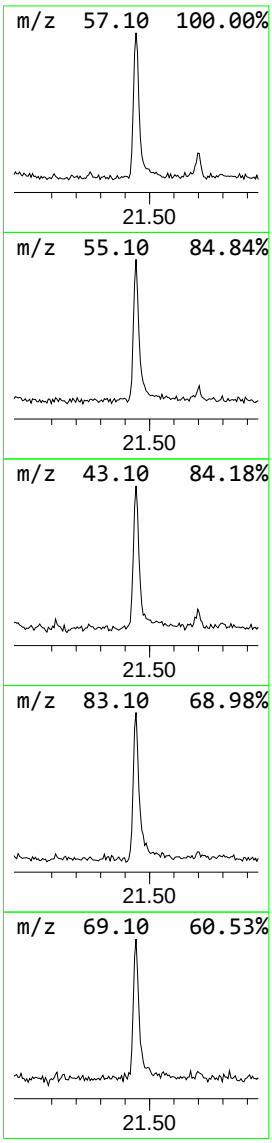
****

Peak Number 9 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.445	4.04 ng	176508	Chrysene-d12	21.827

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	92
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

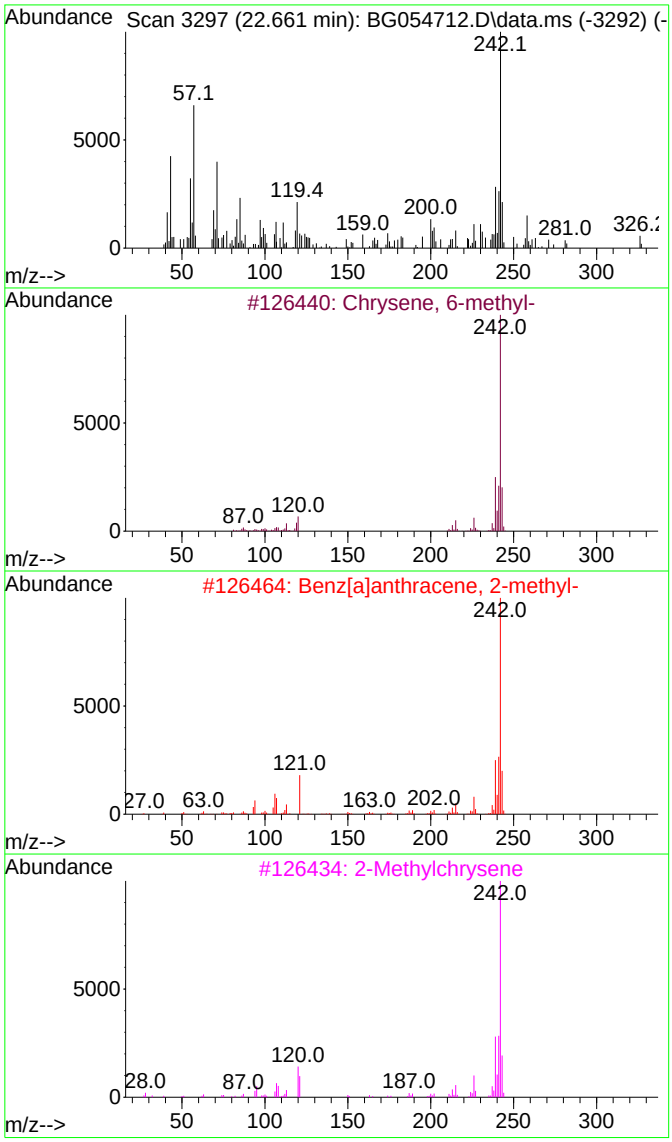
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

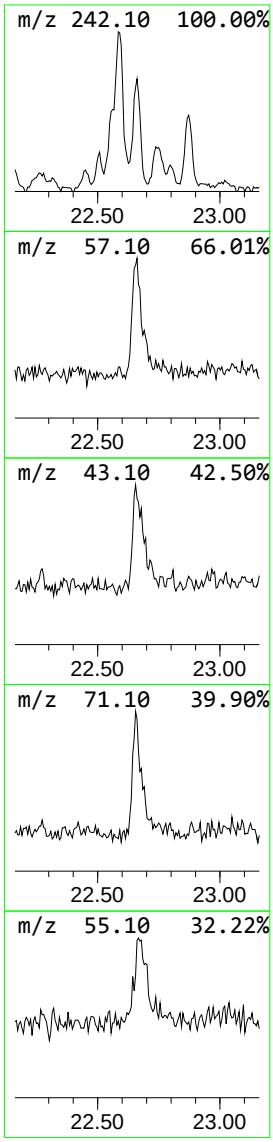
****

Peak Number 10 unknown22.661 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.661	2.22 ng	97071	Chrysene-d12	21.827

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chrysene, 6-methyl-	242	C19H14	001705-85-7	46
2	Benz[a]anthracene, 2-methyl-	242	C19H14	002498-76-2	46
3	2-Methylchrysene	242	C19H14	003351-32-4	46
4	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	45
5	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

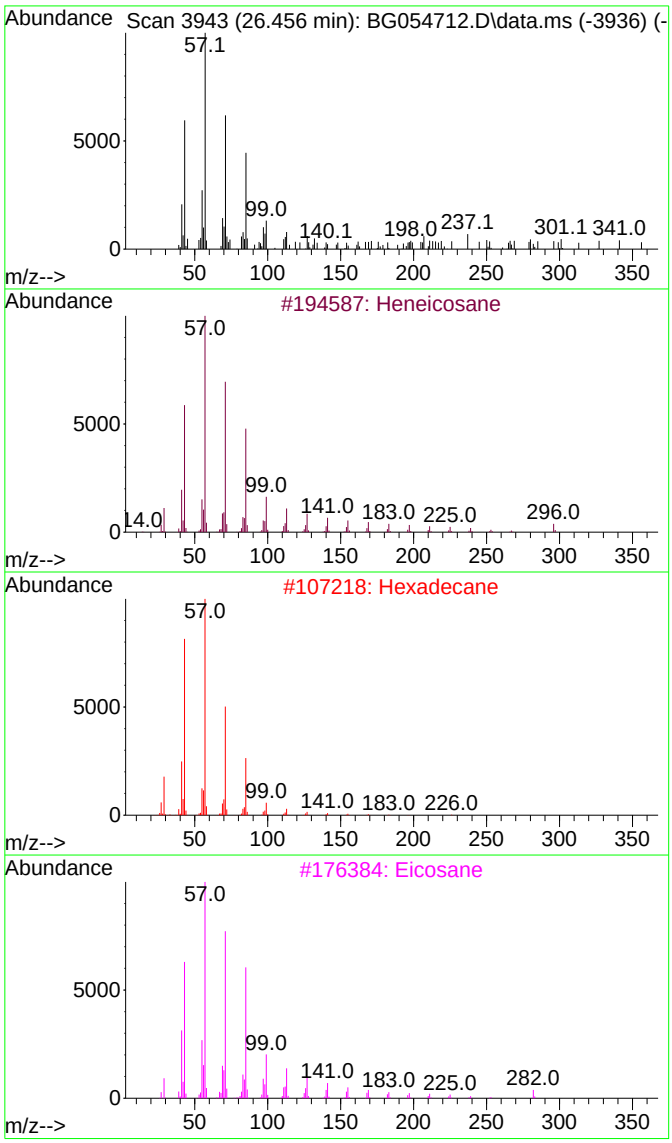
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

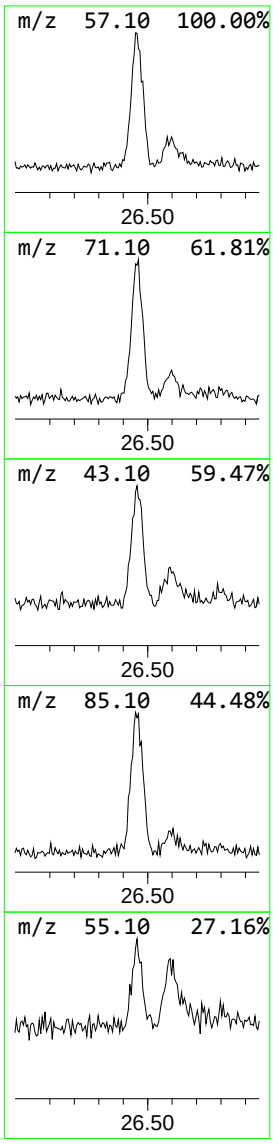
****

Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.456	2.71 ng	104926	Perylene-d12	25.205

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Hexadecane	226	C16H34	000544-76-3	83
3	Eicosane	282	C20H42	000112-95-8	83
4	Tetradecane	198	C14H30	000629-59-4	64
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054712.D
Acq On : 23 Aug 2022 18:19
Operator : CG/JU
Sample : N4274-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.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
unknown3.789	3.789	2.6	ng	43591	1	8.160	337987	20.0
2-Pentanone, 4-...	5.228	7.8	ng	131528	1	8.160	337987	20.0
unknown9.030	9.030	6.2	ng	104708	1	8.160	337987	20.0
Phenanthrene, 1...	18.407	5.7	ng	215805	4	17.538	753059	20.0
Anthracene, 2-m...	18.454	3.3	ng	123183	4	17.538	753059	20.0
Phenanthrene, 2...	18.595	2.8	ng	105368	4	17.538	753059	20.0
1H-Cyclopropa[l...	18.636	2.1	ng	78453	4	17.538	753059	20.0
Phenanthrene, 2...	19.318	3.2	ng	119455	4	17.538	753059	20.0
1-Octadecene	21.445	4.0	ng	176508	5	21.827	874244	20.0
unknown22.661	22.661	2.2	ng	97071	5	21.827	874244	20.0
Heneicosane	26.456	2.7	ng	104926	6	25.205	774001	20.0