LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-VNJ-209

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_P\Methods\8270E-BP031722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.881	317	322	330	rVB	85710	146380	1.23%	0.173%
2	5.346	395	401	431	rBV	3789598	6810646	57.34%	8.036%
3	6.934	661	671	688	rBV	3726591	6996768	58.91%	8.256%
4	7.740	801	808	817	rBV	935947	1617037	13.61%	1.908%
5	8.899	998	1005	1030	rVB	2462395	4610404	38.82%	5.440%
6	10.534	1274	1283	1289	rBV	1242757	2407159	20.27%	2.840%
7	13.010	1696	1704	1717	rBV	4513916	7393391	62.25%	8.724%
8	14.110	1885	1891	1903	rBV	150362	271645	2.29%	0.321%
9	14.392	1931	1939	1945	rBV	1567979	2544195	21.42%	3.002%
10	14.451	1945	1949	1961	rVB	165027	278879	2.35%	0.329%
11	14.792	2002	2007	2013	rBV	91871	150570	1.27%	0.178%
12	15.445	2112	2118	2128	rBV2	198927	360021	3.03%	0.425%
13	15.892	2187	2194	2213	rBV	5027372	8102202	68.21%	9.560%
14	16.128	2229	2234	2242	rVB5	61693	128481	1.08%	0.152%
15	16.975	2374	2378	2388	rVB	94218	165525	1.39%	0.195%
16	17.157	2402	2409	2413	rBV	2418342	3795630	31.96%	4.479%
17	17.198	2413	2416	2424	rVV	1353604	1994665	16.79%	2.354%
18	17.292	2427	2432	2438	rVB	295279	469574	3.95%	0.554%
19	17.569	2474	2479	2489	rBV	92548	185908	1.57%	0.219%
20	18.033	2553	2558	2560	rBV	166061	236858	1.99%	0.279%
21	18.069	2560	2564	2573	rVB2	521243	972182	8.18%	1.147%
22	18.222	2585	2590	2594	rBV2	298444	522881	4.40%	0.617%
23	18.475	2629	2633	2637	rBV	306503	390099	3.28%	0.460%
24	18.522	2637	2641	2645	rVV	130074	191365	1.61%	0.226%
25	18.569	2645	2649	2658	rVB	114970	200725	1.69%	0.237%
26	18.898	2700	2705	2715	rBV2	643692	1198809	10.09%	1.415%
27	19.069	2730	2734	2740	rVB2	103022	166130	1.40%	0.196%
28	19.186	2748	2754	2761	rBV	2274117	3416887	28.77%	4.032%
29	19.539	2805	2814	2823	rBV	1896250	3333903	28.07%	3.934%
30	19.739	2842	2848	2853	rBV	8828160	11877639	100.00%	14.015%
31	20.022	2893	2896	2904	rVB	348185	527639	4.44%	0.623%
32	20.122	2910	2913	2917	rBV	222391	272904	2.30%	0.322%
33	20.986	3057	3060	3068	rVB4	765885	1227091	10.33%	1.448%
34	21.274	3103	3109	3113	rBV2	3093794	5241845	44.13%	6.185%
35	21.310	3113	3115	3121	rVB	950863	1133058	9.54%	1.337%
36	22.939	3387	3392	3397	rBV	880274	1955586	16.46%	2.308%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

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_P\Methods\8270E-BP031722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.662	3509	3515	3521	rBV	1760638	3452955	29.07%	4.074%

Sum of corrected areas: 84747636

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
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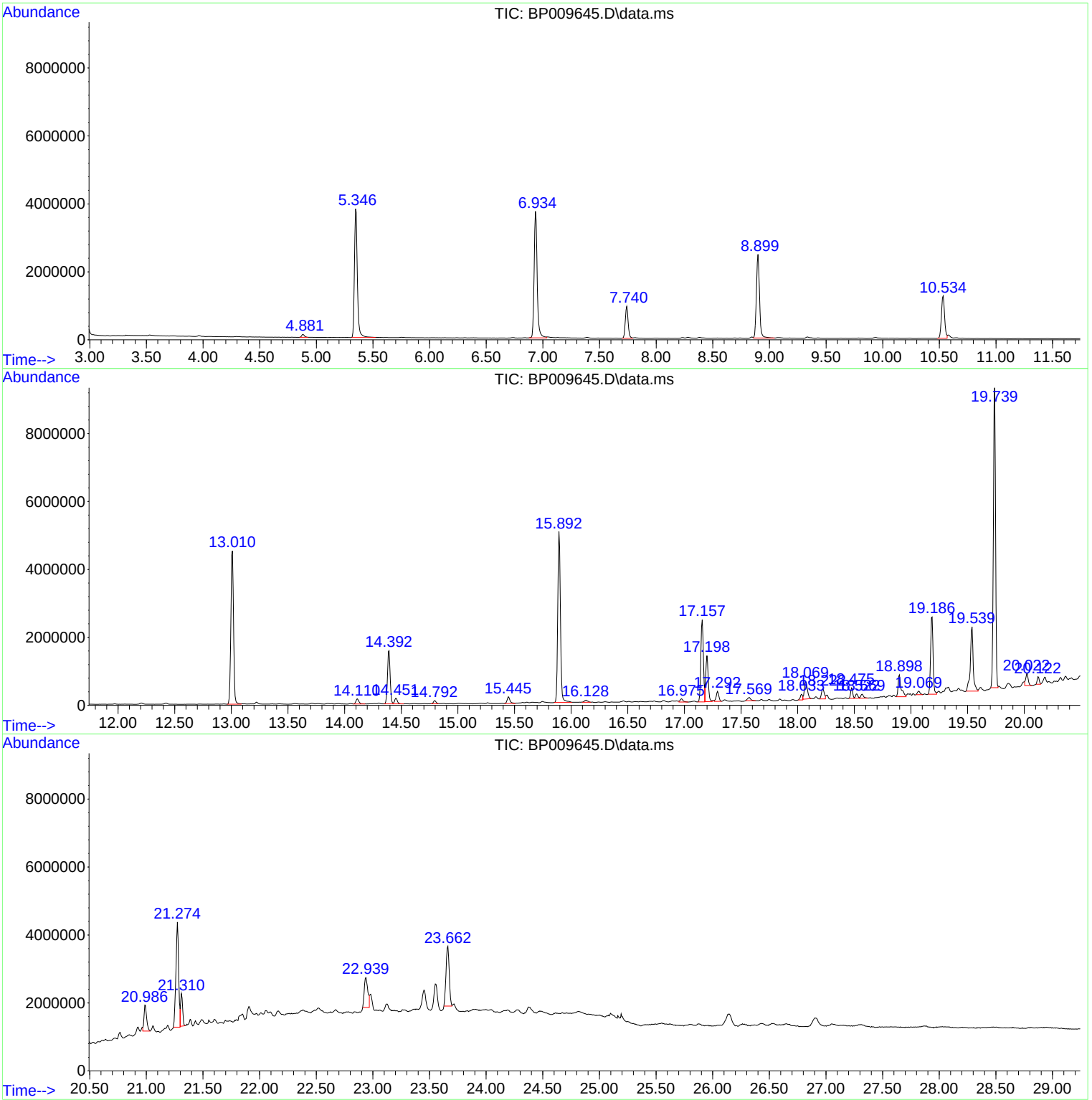
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.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_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

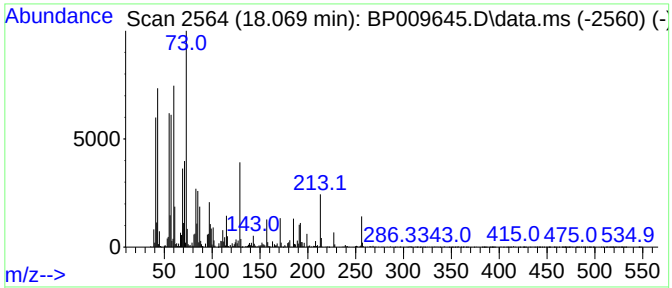
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

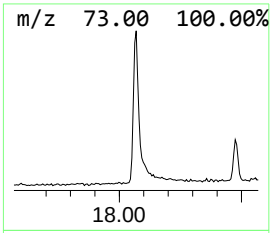
****

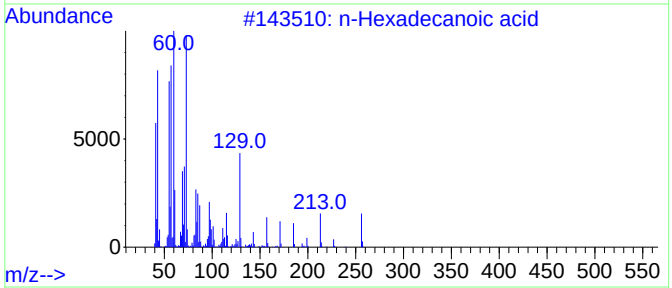
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

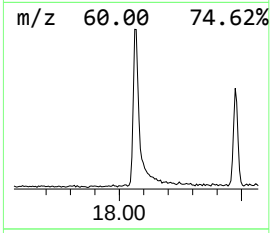
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	5.12 ng	972182	Phenanthrene-d10	17.157

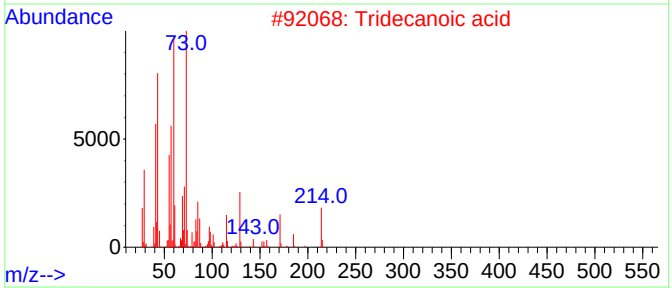
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81

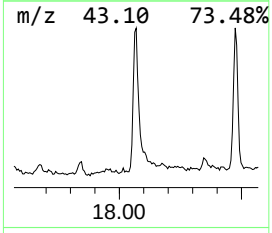


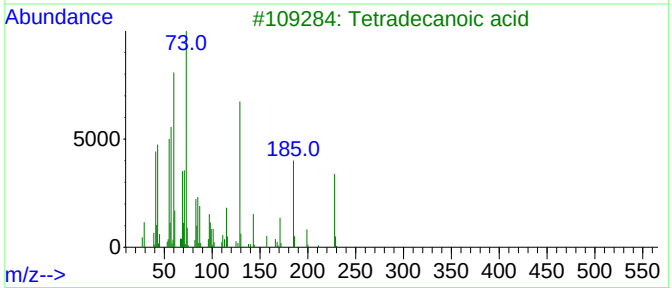


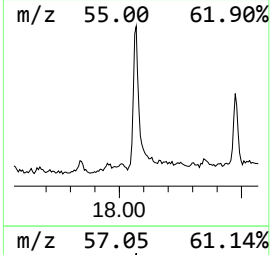


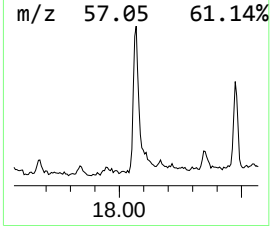












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

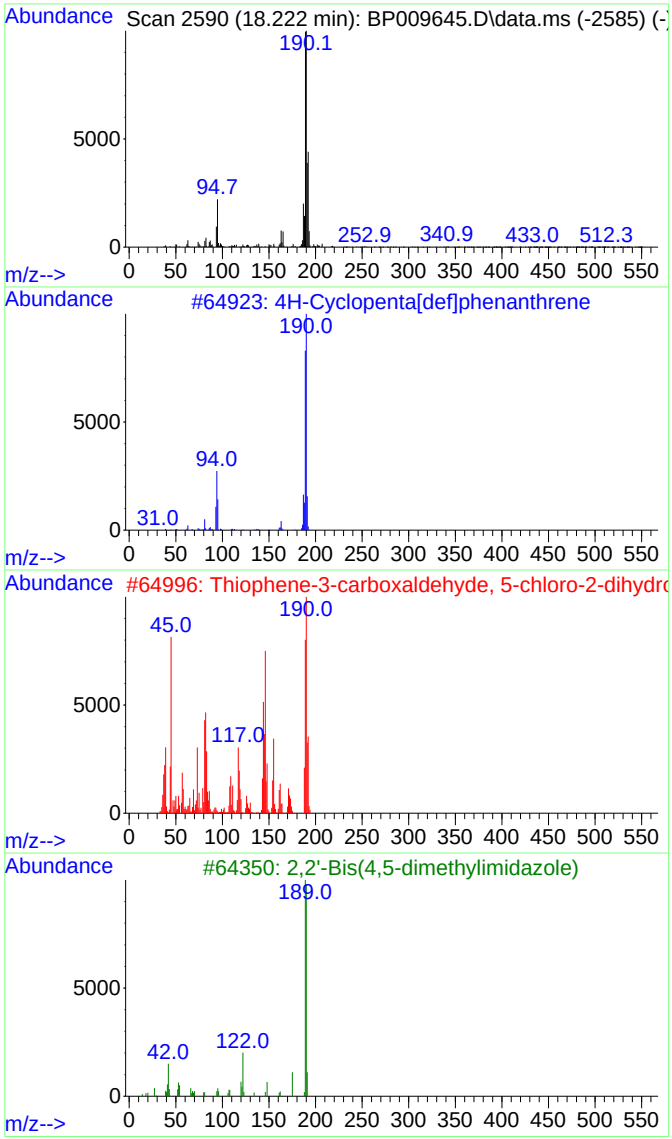
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

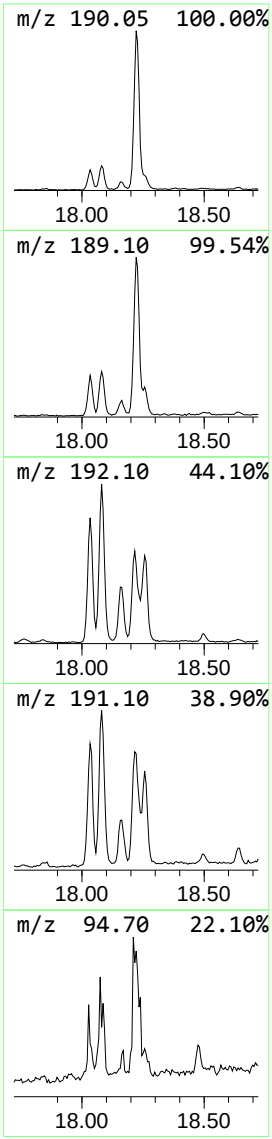
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	2.76 ng	522881	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

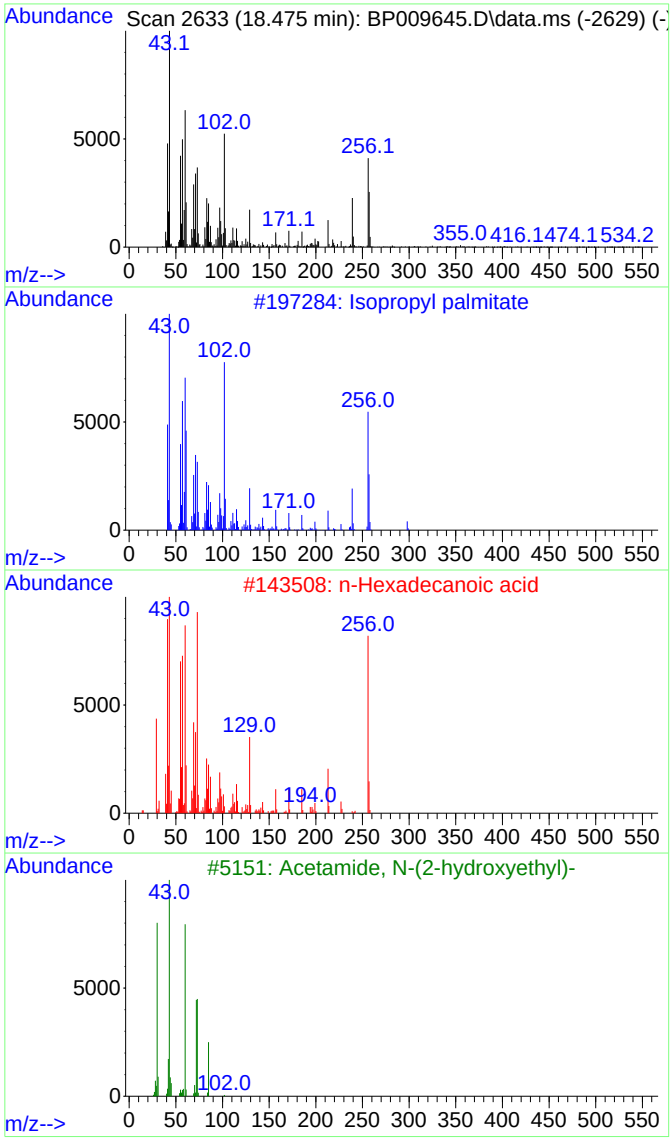
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

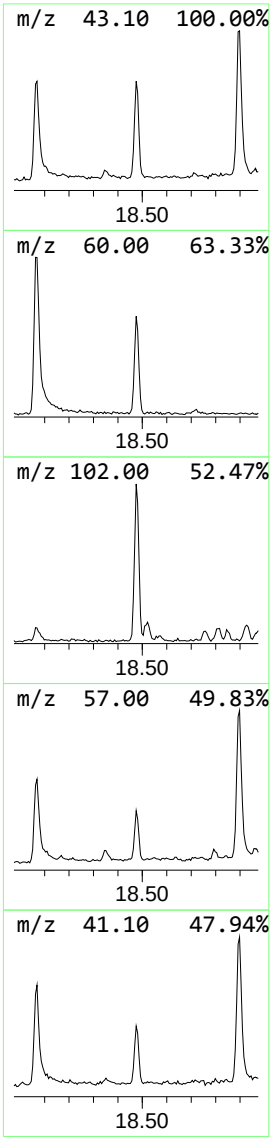
****

Peak Number 4 Isopropyl palmitate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.474	2.06 ng	390099	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	83
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42
3	Acetamide, N-(2-hydroxyethyl)-	103	C4H9NO2	000142-26-7	22
4	3,4-Altrosan	162	C6H10O5	1000129-76-4	22
5	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

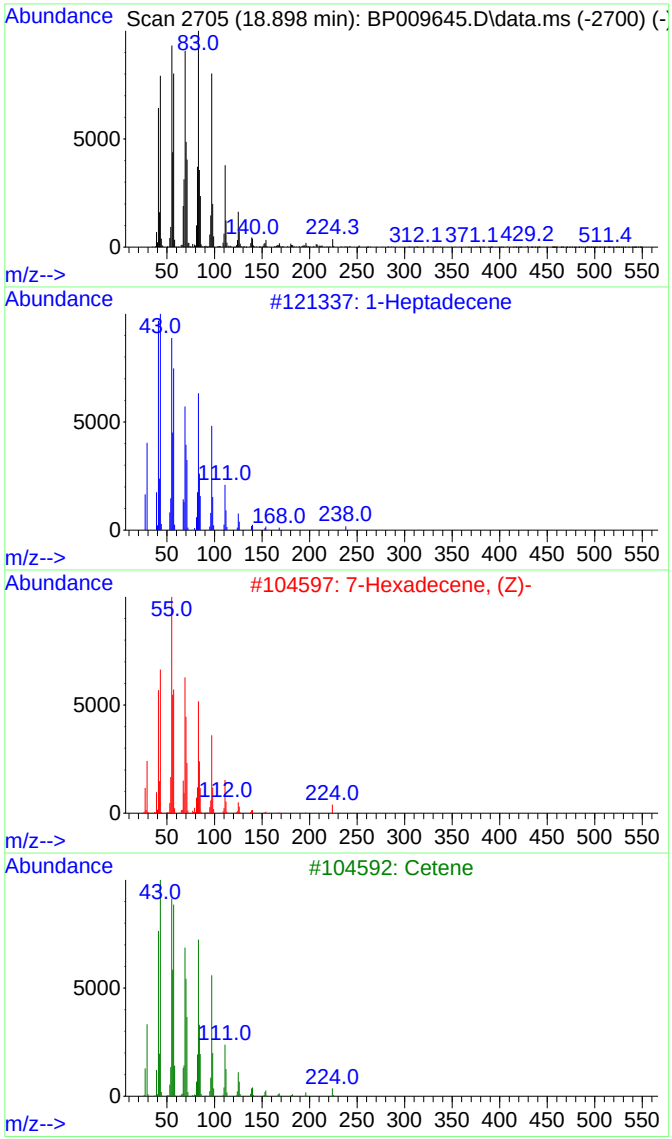
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

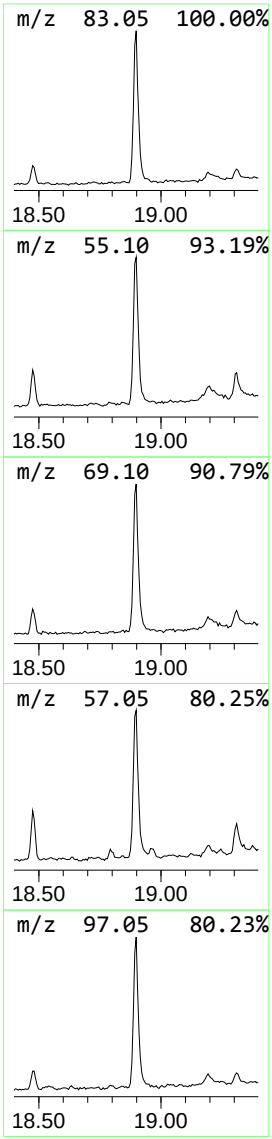
****

Peak Number 5 1-Heptadecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.898	6.32 ng	1198810	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	99
2	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	96
3	Cetene	224	C16H32	000629-73-2	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

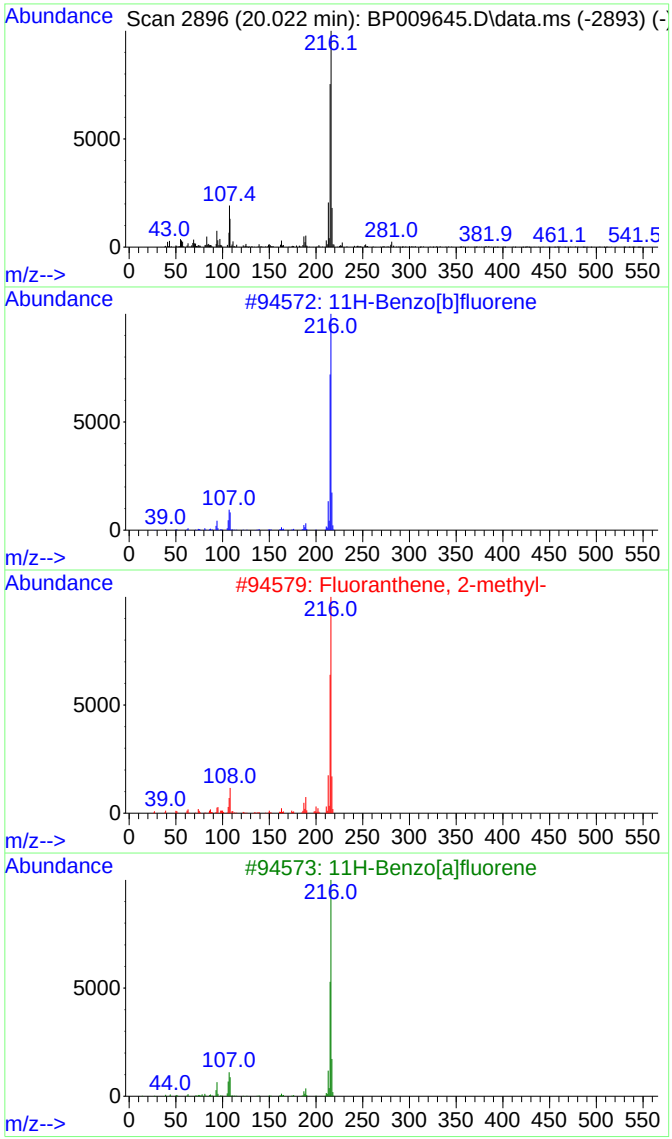
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

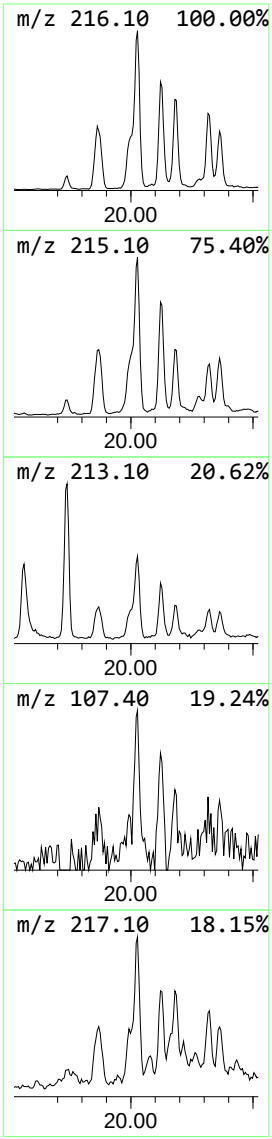
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.022	2.01 ng	527639	Chrysene-d12	21.274

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	80
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

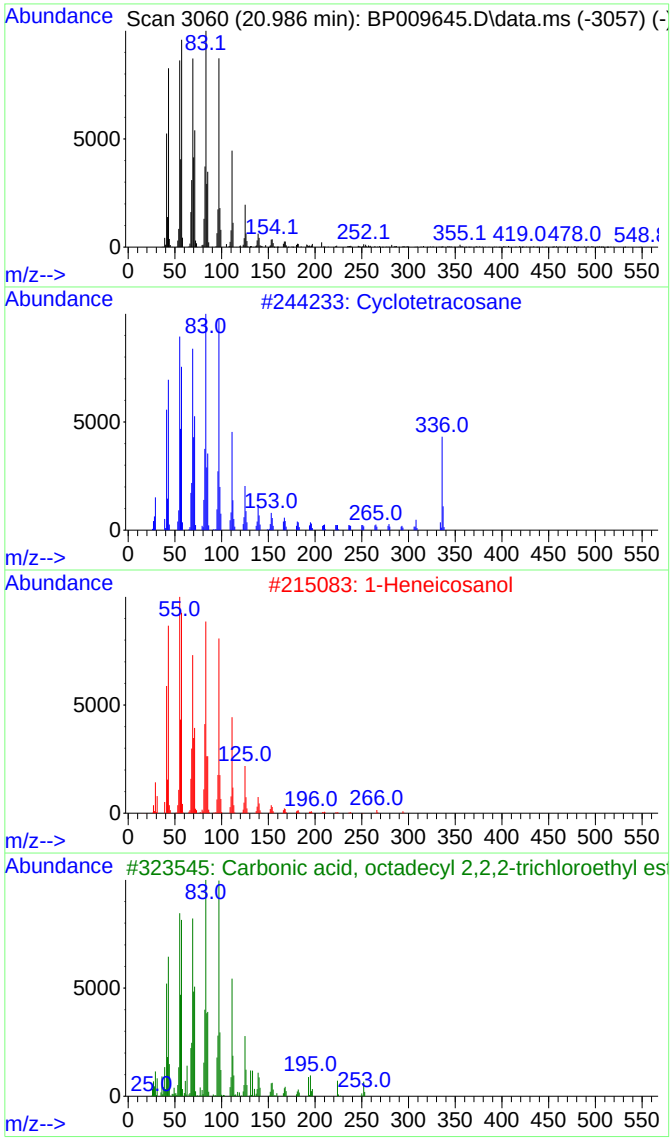
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

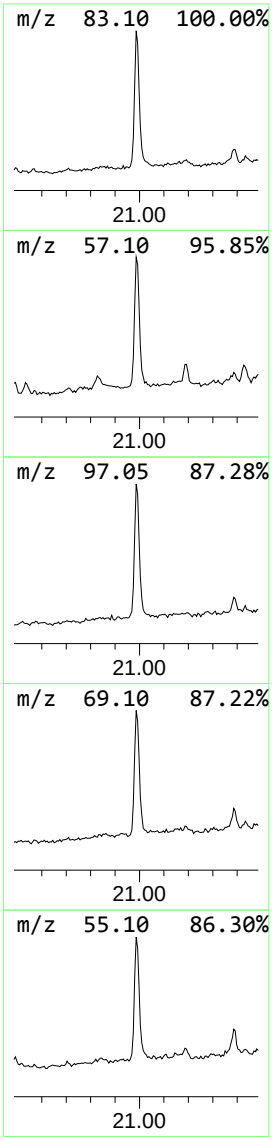
****

Peak Number 7 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	4.68 ng	1227090	Chrysene-d12	21.274

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033122\
Data File : BP009645.D
Acq On : 31 Mar 2022 18:24
Operator : CG/JU
Sample : N2199-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-VNJ-209

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.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
n-Hexadecanoic ...	18.069	5.1	ng	972182	4	17.157	3795630	20.0
4H-Cyclopenta[d...	18.222	2.8	ng	522881	4	17.157	3795630	20.0
Isopropyl palmi...	18.474	2.1	ng	390099	4	17.157	3795630	20.0
1-Heptadecene	18.898	6.3	ng	1198810	4	17.157	3795630	20.0
11H-Benzo[b]flu...	20.022	2.0	ng	527639	5	21.274	5241850	20.0
Cyclotetracosane	20.986	4.7	ng	1227090	5	21.274	5241850	20.0