LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

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-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.064	8	13	25	rVB	168119	292541	3.10%	0.293%
2	5.422	407	414	431	rVB	1542255	2610209	27.62%	2.618%
3	7.005	676	683	695	rBV	1359084	2633675	27.87%	2.641%
4	7.810	810	820	829	rBV	1168291	2033550	21.52%	2.039%
5	8.963	1006	1016	1028	rBV	910315	1742994	18.44%	1.748%
6	10.404	1255	1261	1270	rBV2	41128	108847	1.15%	0.109%
7	10.604	1287	1295	1311	rBV	1503003	2883515	30.51%	2.892%
8	12.393	1592	1599	1613	rBV2	67486	243254	2.57%	0.244%
9	13.075	1708	1715	1729	rBV	2644986	4290653	45.40%	4.303%
10	14.175	1896	1902	1915	rVB	532081	923499	9.77%	0.926%
11	14.316	1920	1926	1932	rBV4	39443	110844	1.17%	0.111%
12	14.451	1942	1949	1957	rBV	2418427	3952674	41.82%	3.964%
13	15.951	2198	2204	2212	rBV	2336284	3672630	38.86%	3.683%
14	16.186	2240	2244	2252	rVB2	83891	149559	1.58%	0.150%
15	16.869	2355	2360	2368	rVB	153848	244239	2.58%	0.245%
16	17.033	2385	2388	2396	rVB	78264	129661	1.37%	0.130%
17	17.216	2413	2419	2423	rBV	2989193	4738729	50.14%	4.752%
18	17.257	2423	2426	2432	rVB	1334867	1885225	19.95%	1.891%
19	17.351	2437	2442	2448	rVV	751030	1210598	12.81%	1.214%
20	17.404	2448	2451	2459	rVB3	90176	169540	1.79%	0.170%
21	17.628	2481	2489	2501	rBV	438710	886694	9.38%	0.889%
22	17.733	2504	2507	2514	rVV5	85949	151286	1.60%	0.152%
23	17.798	2515	2518	2527	rVV8	81615	142717	1.51%	0.143%
24	18.086	2564	2567	2569	rBV	139924	175005	1.85%	0.175%
25	18.122	2569	2573	2581	rVB2	1166397	1897923	20.08%	1.903%
26	18.216	2586	2589	2594	rVB	165561	232642	2.46%	0.233%
27	18.280	2595	2600	2604	rBV2	350736	598645	6.33%	0.600%
28	18.575	2647	2650	2653	rBV	159244	194331	2.06%	0.195%
29	18.610	2653	2656	2662	rVB	336457	449410	4.76%	0.451%
30	18.986	2716	2720	2724	rBV2	225358	330734	3.50%	0.332%
31	19.110	2737	2741	2749	rVB2	468868	807952	8.55%	0.810%
32	19.239	2757	2763	2770	rBV	4658191	7007434	74.14%	7.027%
33	19.380	2780	2787	2792	rBV2	822142	1785174	18.89%	1.790%
34	19.592	2818	2823	2831	rVB	3719339	5405794	57.20%	5.421%
35	19.792	2852	2857	2868	rVB	4336619	6794966	71.90%	6.814%
36	20.810	3027	3030	3035	rBV	770748	1065837	11.28%	1.069%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

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-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.016	3062	3065	3068	rBV2	470816	630483	6.67%	0.632%
38	21.051	3068	3071	3076	rVV2	756839	1113010	11.78%	1.116%
39	21.104	3077	3080	3084	rBV	746843	998851	10.57%	1.002%
40	21.321	3111	3117	3121	rBV3	4910270	9451184	100.00%	9.478%
41	21.363	3121	3124	3133	rVB	2365905	3324132	35.17%	3.334%
42	21.445	3134	3138	3143	rBV	2492086	3856008	40.80%	3.867%
43	23.010	3398	3404	3409	rBV2	2408251	5936114	62.81%	5.953%
44	23.527	3488	3492	3502	rVB2	1440102	3185475	33.70%	3.194%
45	23.633	3505	3510	3519	rVB	1998838	4054831	42.90%	4.066%
46	23.739	3522	3528	3534	rBV2	2385173	5215003	55.18%	5.230%

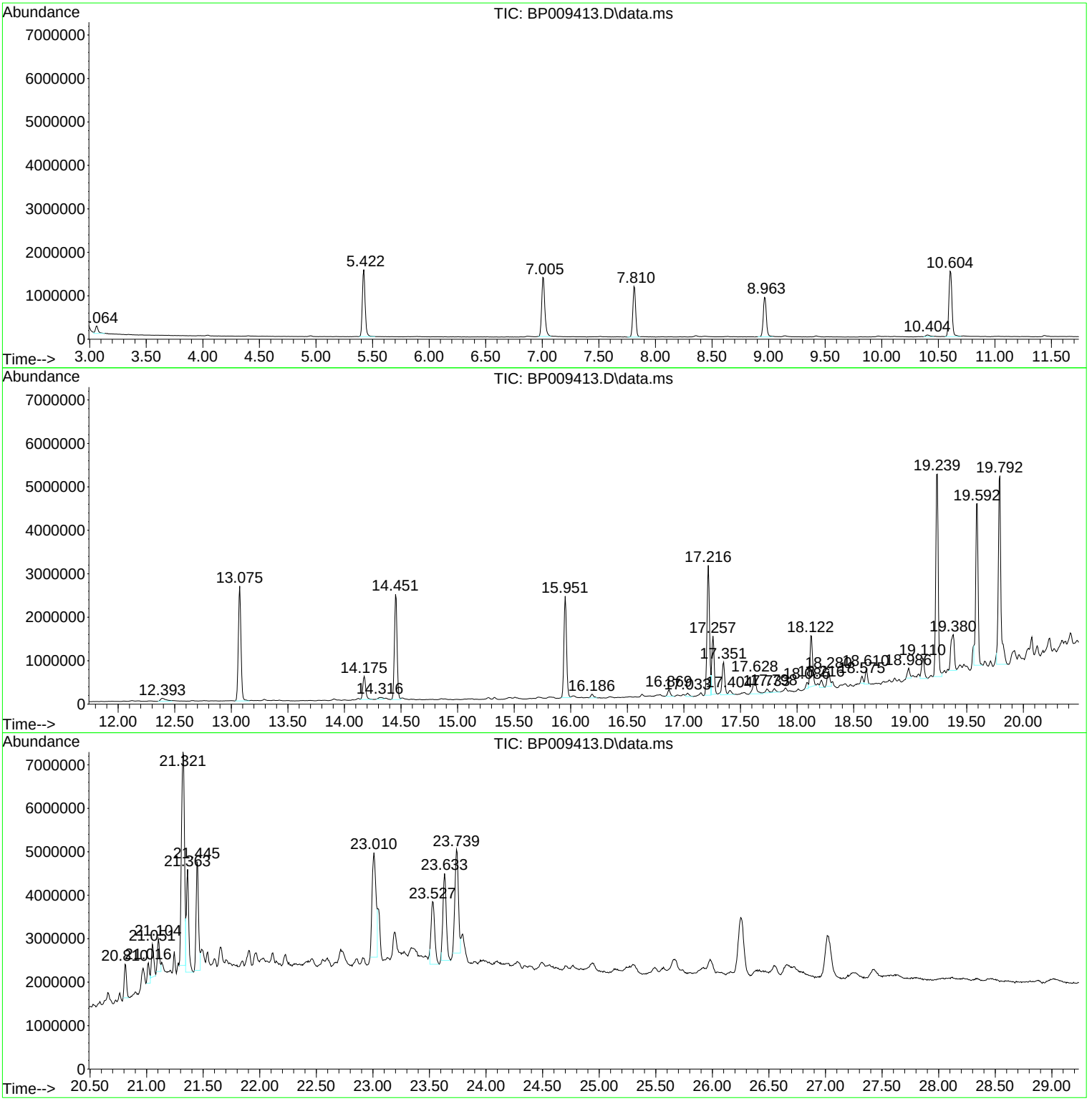
Sum of corrected areas: 99718071

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

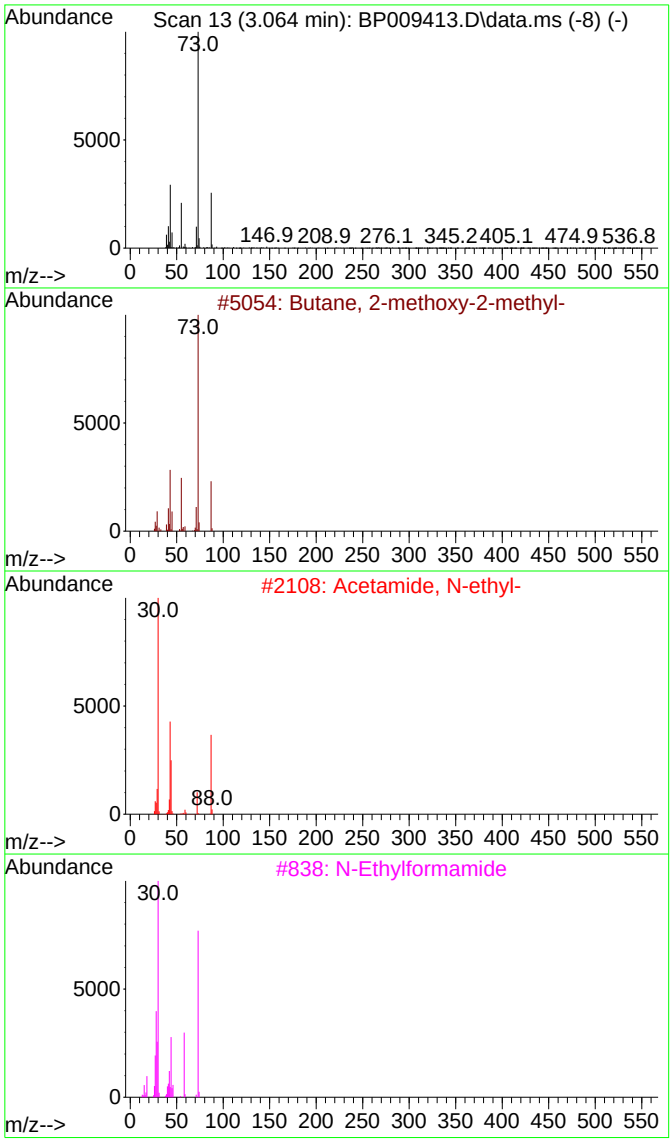
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

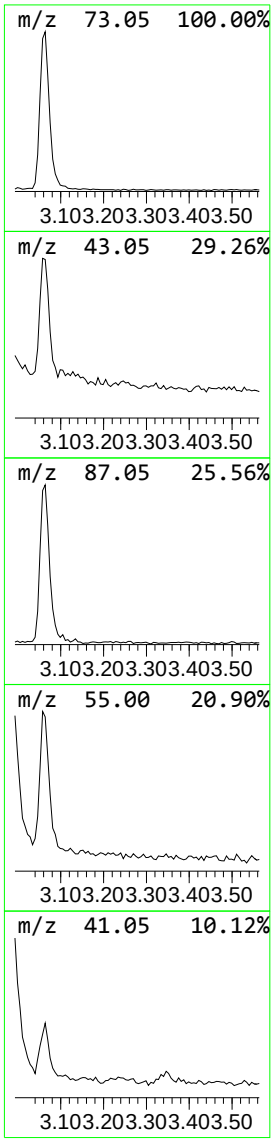
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.064	2.88 ng	292541	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

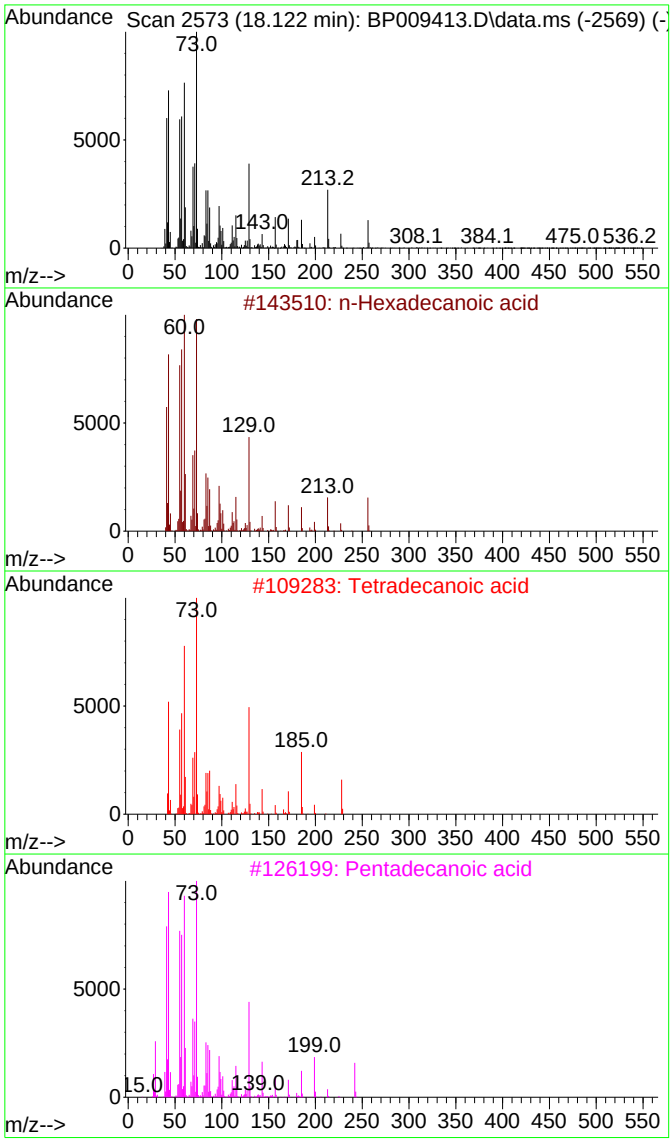
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

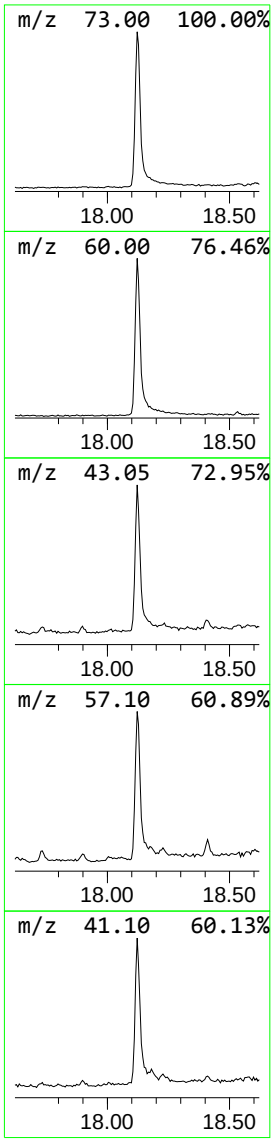
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	8.01 ng	1897920	Phenanthrene-d10	17.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

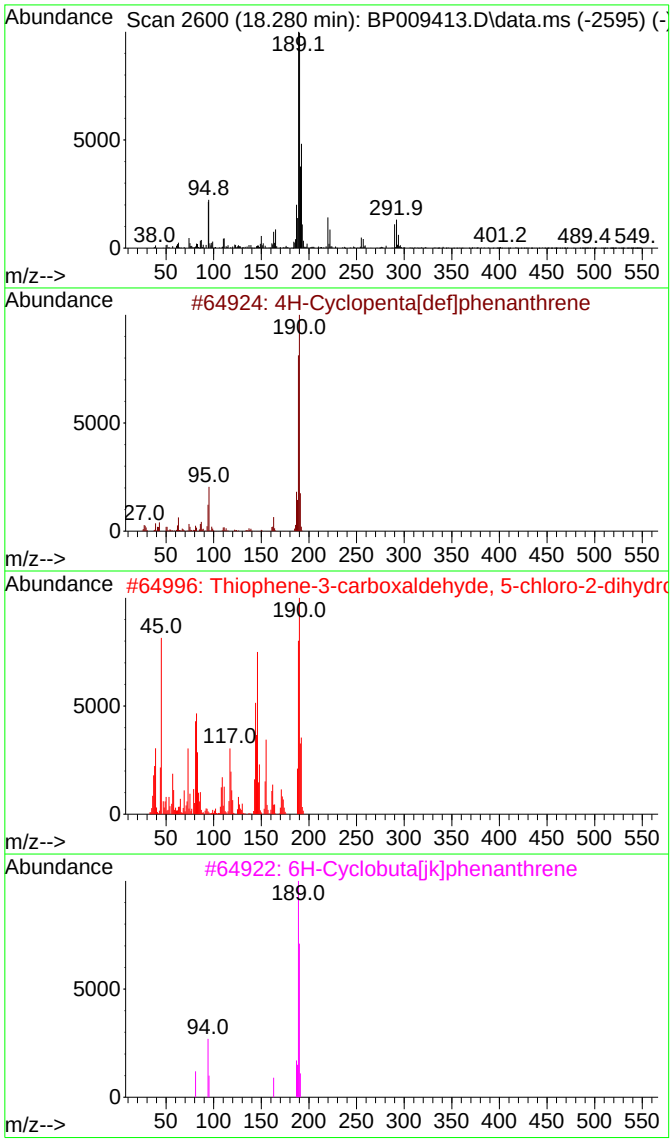
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

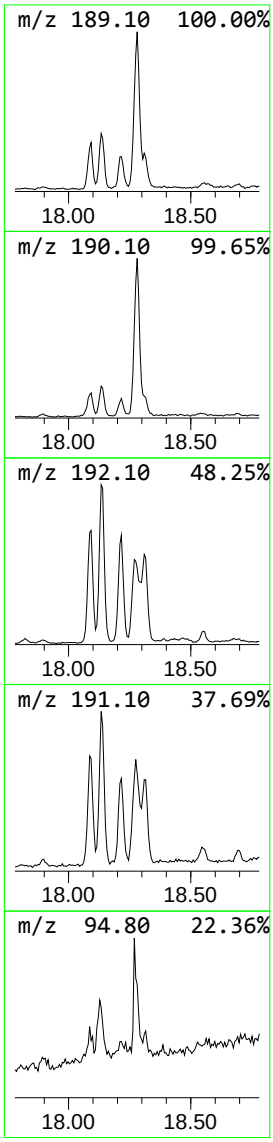
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.280	2.53 ng	598645	Phenanthrene-d10	17.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	64
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
5	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

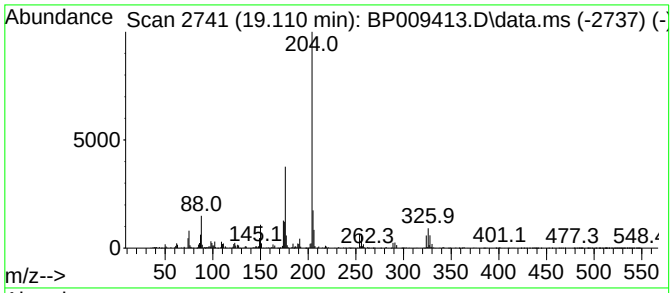
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

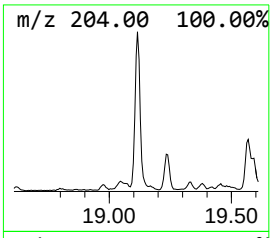
****

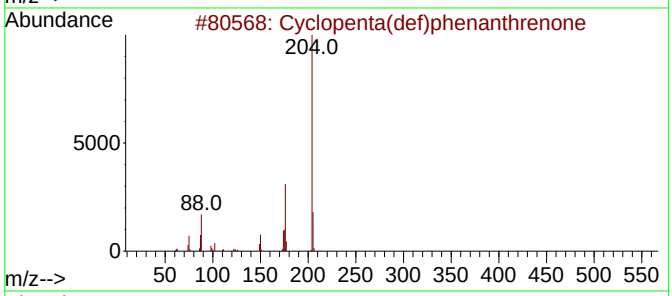
Peak Number 4 Cyclopenta(def)phenanthrenone Concentration Rank 5

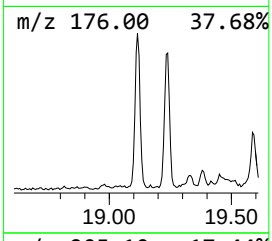
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.110	3.41 ng	807952	Phenanthrene-d10	17.216

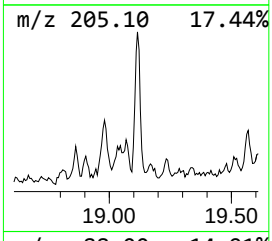
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	96
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	64
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	50
4	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	49
5	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	47

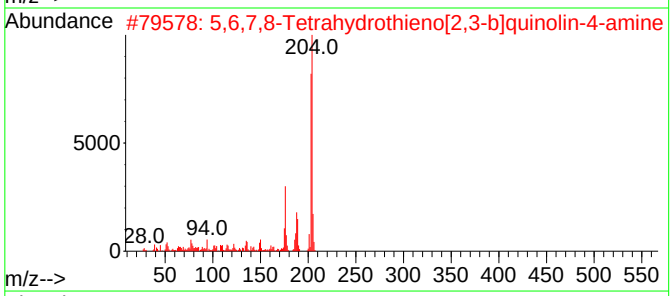


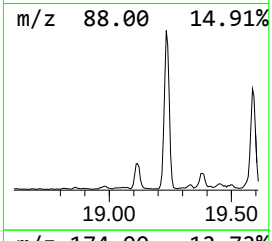


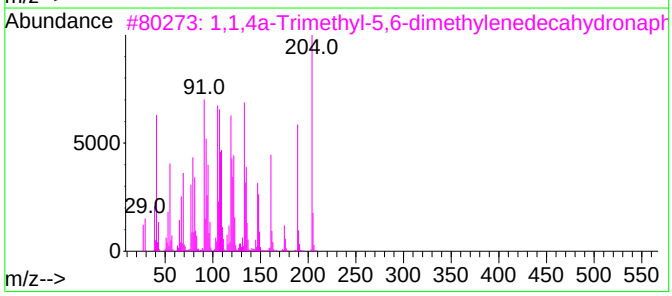


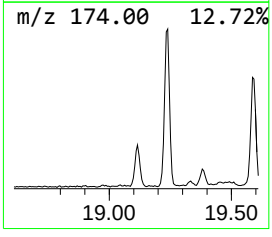












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

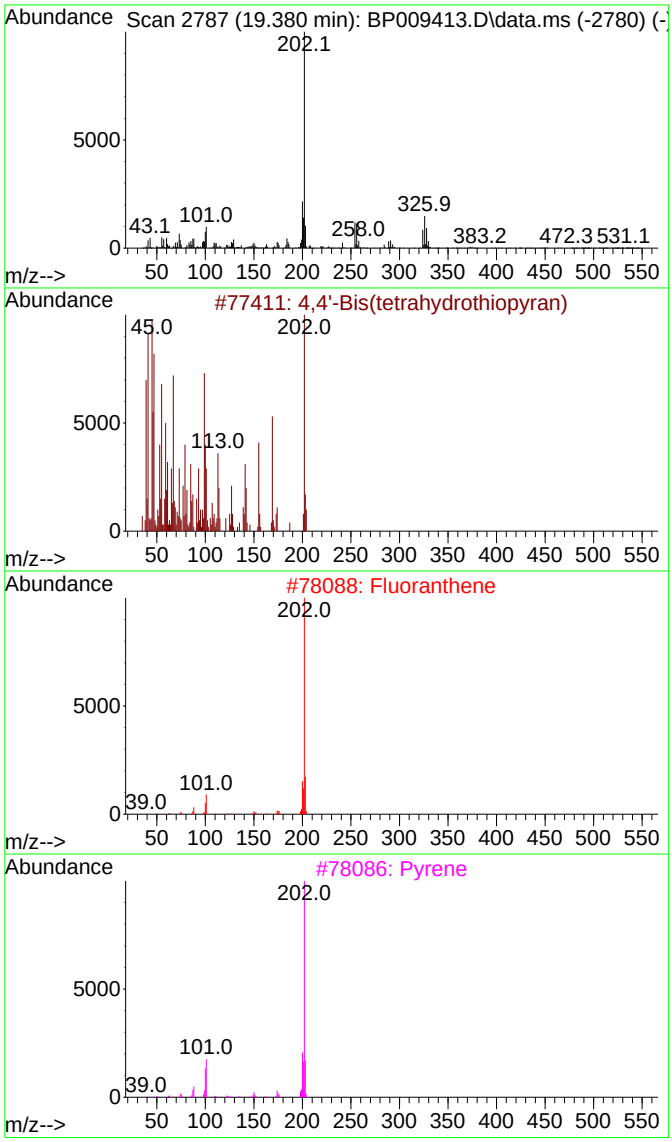
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

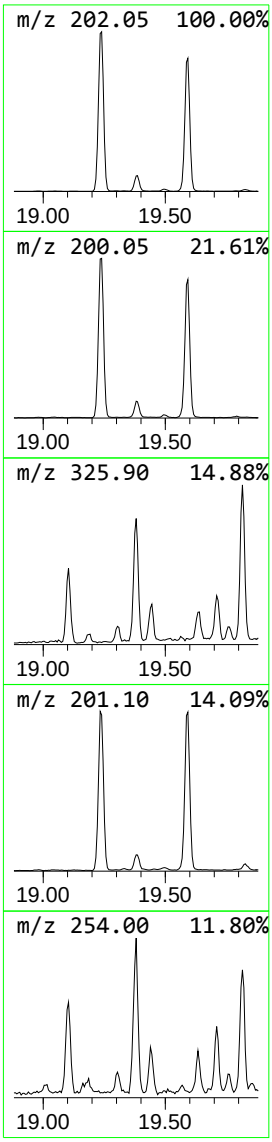
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.380	3.78 ng	1785170	Chrysene-d12	21.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	94
2	Fluoranthene	202	C16H10	000206-44-0	50
3	Pyrene	202	C16H10	000129-00-0	50
4	benzenesulfonamide, N-(4,5-dihyd...	343	C17H17N3O3S	1000398-24-4	38
5	3-Trifluoromethylbenzylamine, N-...	329	C19H30F3N	1000310-29-2	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

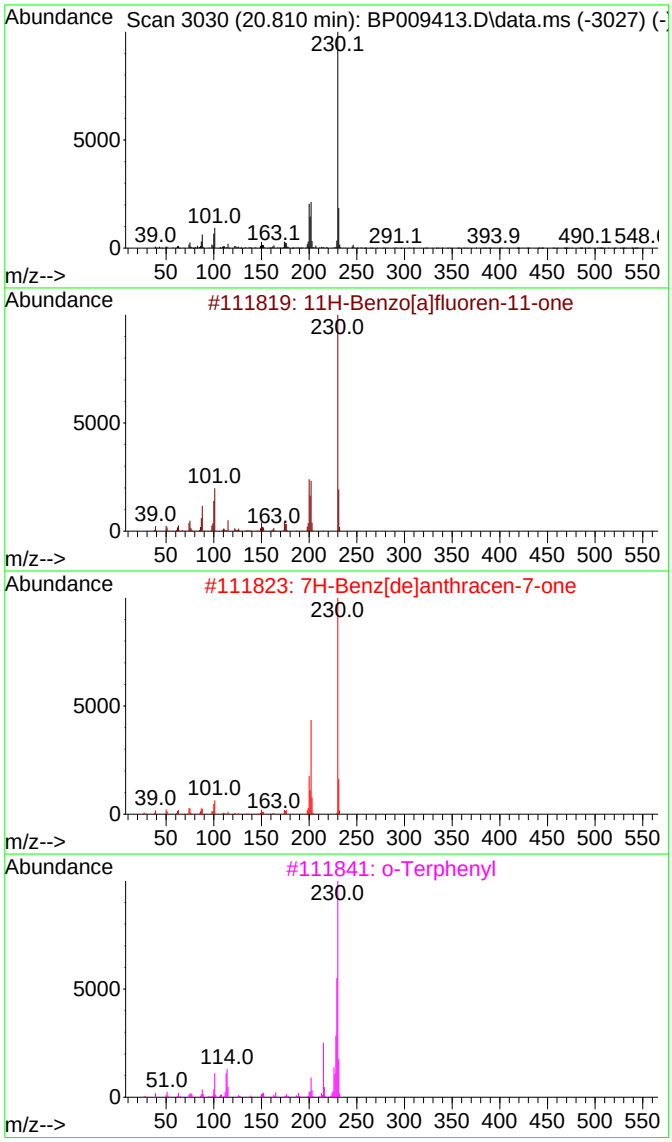
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

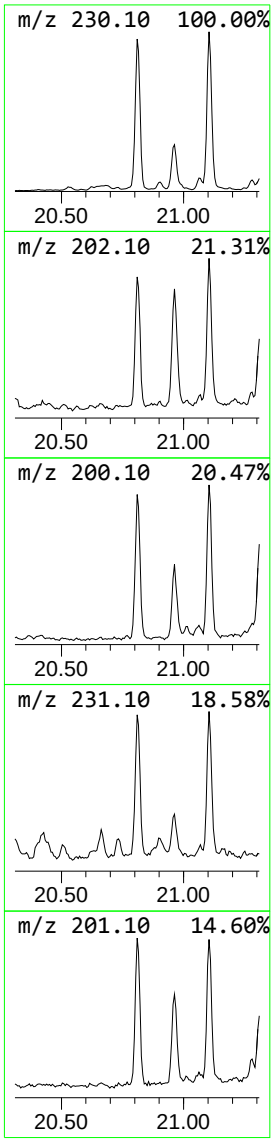
****

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.810	2.26 ng	1065840	Chrysene-d12	21.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	97
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	90
3	o-Terphenyl	230	C18H14	000084-15-1	58
4	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	53
5	Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

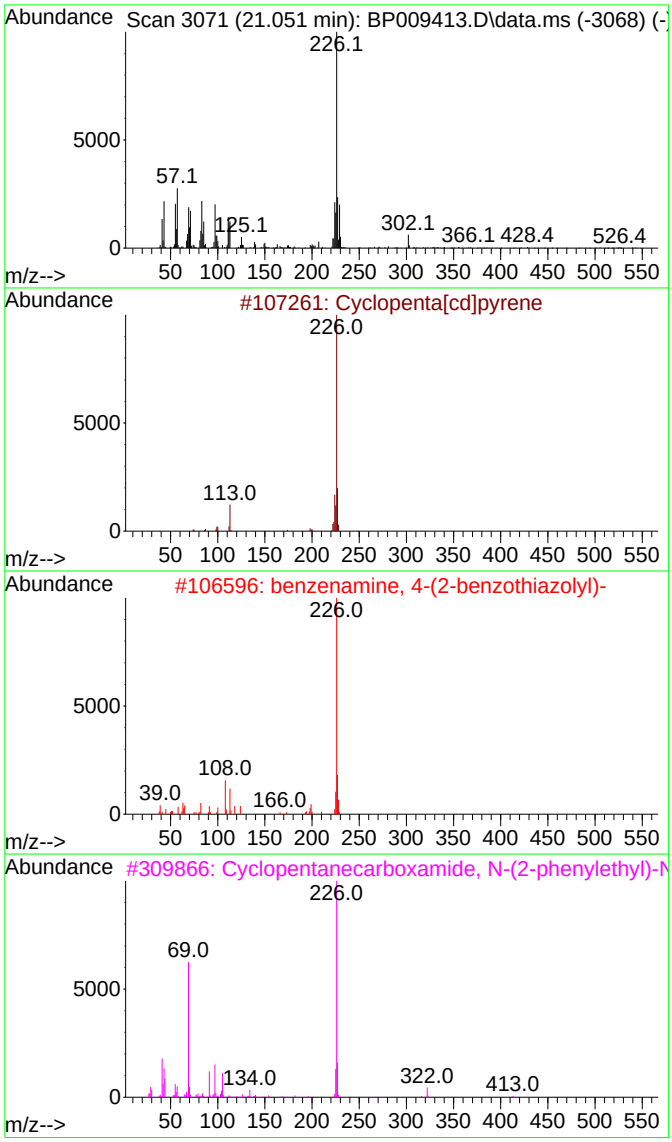
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

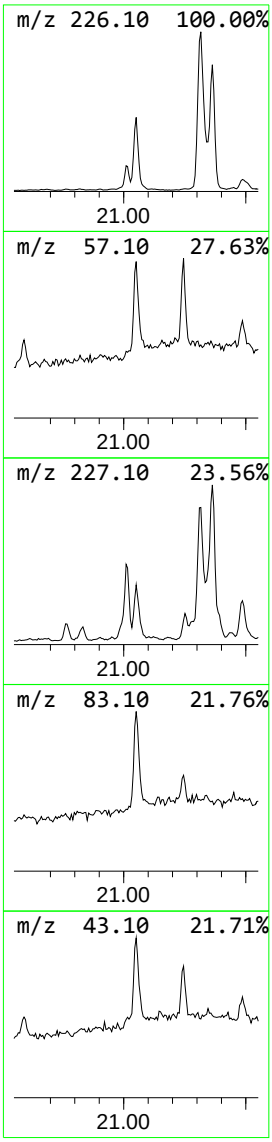
****

Peak Number 7 Cyclopenta[cd]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	2.36 ng	1113010	Chrysene-d12	21.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	91
2	benzenamine, 4-(2-benzothiazolyl)-	226	C13H10N2S	1000400-93-4	47
3	Cyclopentanecarboxamide, N-(2-ph...	413	C28H47NO	1000451-59-7	42
4	9H-Thioxanthen-9-one, 2-methyl-	226	C14H10OS	015774-82-0	38
5	Benzonitrile, 2-(5-methyl-2-thie...	226	C13H10N2S	315670-19-0	28





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Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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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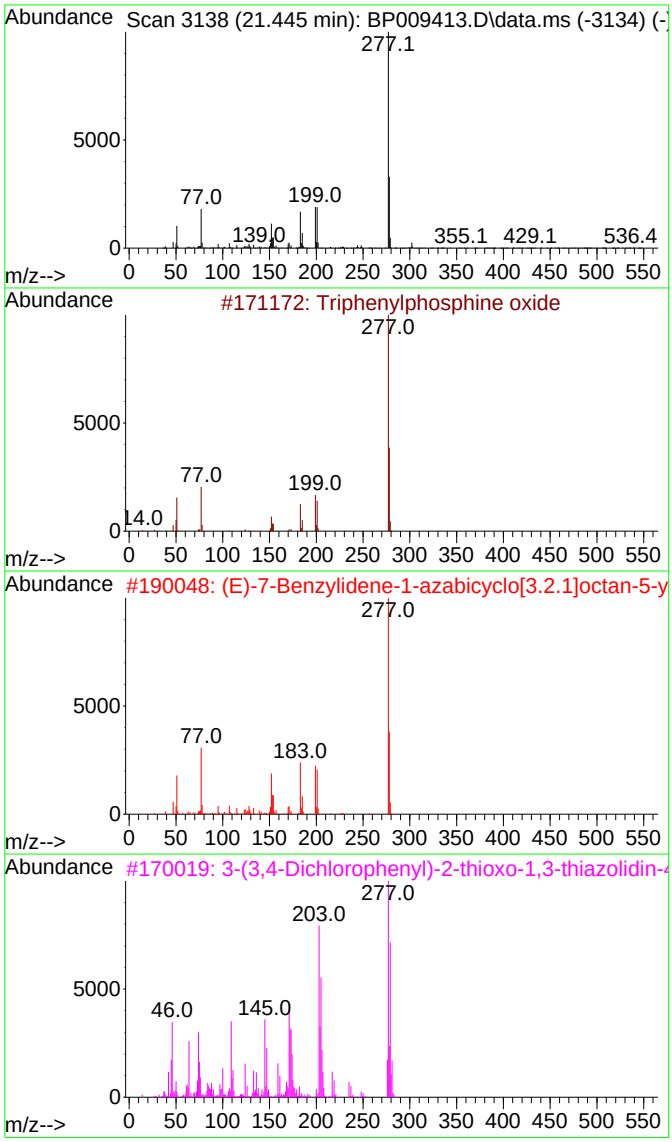
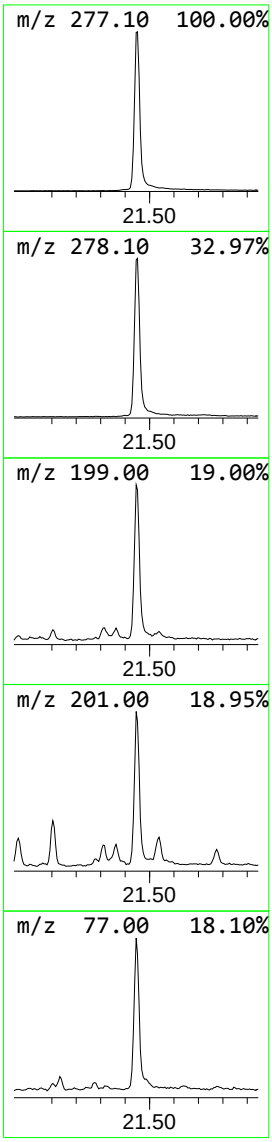
Peak Number 9 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.445	8.16 ng	3856010	Chrysene-d12	21.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
3	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	38
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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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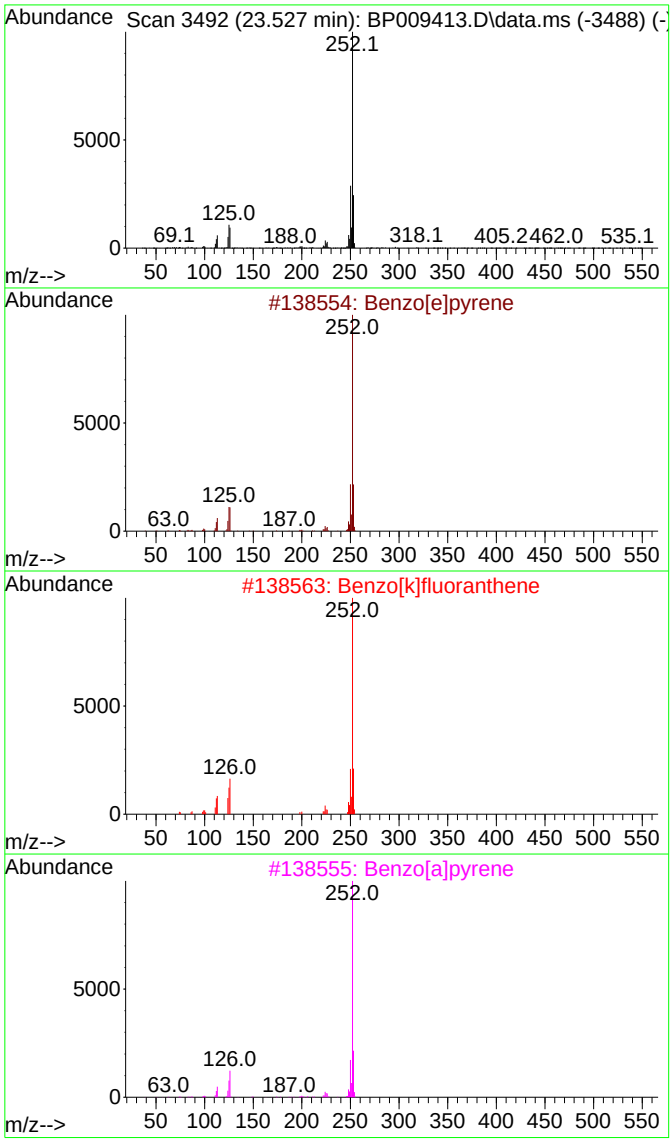
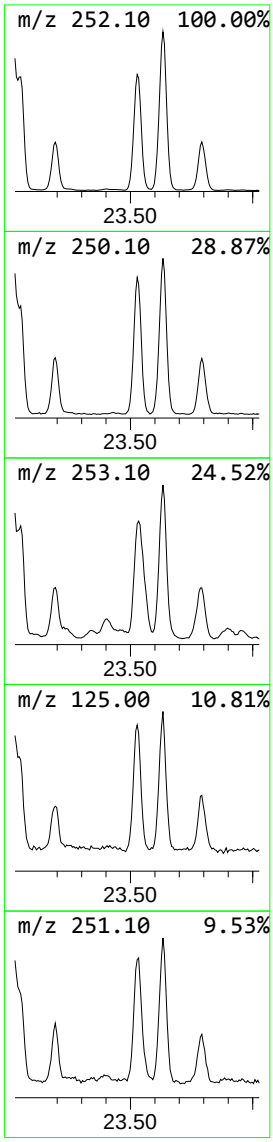
Peak Number 10 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.527	12.22 ng	3185480	Perylene-d12	23.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031522\
Data File : BP009413.D
Acq On : 15 Mar 2022 23:35
Operator : CG/JU
Sample : N1894-05 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP5(0-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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
Butane, 2-metho...	3.064	2.9	ng	292541	1	7.810	2033550	20.0
n-Hexadecanoic ...	18.122	8.0	ng	1897920	4	17.216	4738730	20.0
4H-Cyclopenta[d...	18.280	2.5	ng	598645	4	17.216	4738730	20.0
Cyclopenta(def)...	19.110	3.4	ng	807952	4	17.216	4738730	20.0
4,4'-Bis(tetrah...	19.380	3.8	ng	1785170	5	21.327	9451180	20.0
11H-Benzo[a]flu...	20.810	2.3	ng	1065840	5	21.327	9451180	20.0
Cyclopenta[cd]p...	21.051	2.4	ng	1113010	5	21.327	9451180	20.0
Triphenylphosph...	21.445	8.2	ng	3856010	5	21.327	9451180	20.0
Benzo[e]pyrene	23.527	12.2	ng	3185480	6	23.739	5215000	20.0