LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	61	64	72	rVB	48940	72214	1.08%	0.077%
2	4.569	279	286	295	rBV	201810	283180	4.23%	0.303%
3	5.016	356	362	376	rBV	3250032	4686679	69.98%	5.021%
4	6.575	619	627	639	rBV	3157170	5014216	74.88%	5.372%
5	6.681	639	645	657	rVB	103096	177828	2.66%	0.191%
6	6.999	694	699	706	rBV	36622	72518	1.08%	0.078%
7	7.363	753	761	770	rVB	944173	1461827	21.83%	1.566%
8	8.510	947	956	966	rBV	1886619	3038006	45.37%	3.255%
9	8.740	990	995	1003	rVB	74943	120289	1.80%	0.129%
10	9.087	1049	1054	1062	rVB	82424	128272	1.92%	0.137%
11	10.116	1221	1229	1244	rVB	1218984	2017793	30.13%	2.162%
12	10.881	1352	1359	1369	rBV	162794	323260	4.83%	0.346%
13	12.628	1649	1656	1668	rBV	3602800	5366376	80.13%	5.749%
14	13.910	1864	1874	1879	rBV2	45830	126244	1.89%	0.135%
15	14.022	1886	1893	1899	rBV	1875364	2763517	41.27%	2.961%
16	14.086	1899	1904	1914	rVB	211816	326914	4.88%	0.350%
17	14.263	1927	1934	1935	rBV	1175641	1689613	25.23%	1.810%
18	14.280	1935	1937	1944	rVB	1502910	1638213	24.46%	1.755%
19	14.427	1957	1962	1967	rBV	71645	112354	1.68%	0.120%
20	15.086	2068	2074	2079	rBV	190853	272227	4.07%	0.292%
21	15.386	2120	2125	2129	rBV	48069	71331	1.07%	0.076%
22	15.533	2143	2150	2159	rBV	4542394	6427029	95.97%	6.886%
23	16.098	2239	2246	2251	rBV3	36434	76401	1.14%	0.082%
24	16.233	2265	2269	2276	rVB5	39598	75651	1.13%	0.081%
25	16.445	2301	2305	2313	rVB	86783	147134	2.20%	0.158%
26	16.539	2315	2321	2325	rVV5	55160	118842	1.77%	0.127%
27	16.604	2325	2332	2343	rVB	130398	253431	3.78%	0.272%
28	16.786	2357	2363	2367	rBV	2402031	3517988	52.53%	3.769%
29	16.827	2367	2370	2378	rVV	2173539	3094079	46.20%	3.315%
30	16.921	2378	2386	2393	rVV	513971	755515	11.28%	0.809%
31	16.986	2393	2397	2403	rVB2	74779	123457	1.84%	0.132%
32	17.174	2424	2429	2430	rBV	51305	69584	1.04%	0.075%
33	17.204	2430	2434	2438	rVB	242864	324619	4.85%	0.348%
34	17.316	2449	2453	2459	rBV5	52818	90020	1.34%	0.096%
35	17.374	2459	2463	2471	rVV5	45817	83338	1.24%	0.089%
36	17.504	2482	2485	2491	rVB4	40165	73152	1.09%	0.078%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.598	2496	2501	2505	rBV6	46907	100242	1.50%	0.107%
38	17.668	2508	2513	2517	rVV	224350	349199	5.21%	0.374%
39	17.721	2517	2522	2530	rVV2	1059109	1634113	24.40%	1.751%
40	17.798	2531	2535	2540	rVV2	166425	293919	4.39%	0.315%
41	17.857	2540	2545	2550	rVV2	440258	784415	11.71%	0.840%
42	17.898	2550	2552	2559	rVB	157447	197057	2.94%	0.211%
43	18.180	2595	2600	2603	rBV	197931	266813	3.98%	0.286%
44	18.221	2603	2607	2611	rVB	243128	306901	4.58%	0.329%
45	18.427	2639	2642	2647	rVB4	54909	70355	1.05%	0.075%
46	18.480	2647	2651	2654	rVB3	64474	85533	1.28%	0.092%
47	18.521	2655	2658	2662	rVB2	60770	71670	1.07%	0.077%
48	18.604	2667	2672	2678	rBV2	133013	253763	3.79%	0.272%
49	18.668	2680	2683	2685	rBV2	53367	69958	1.04%	0.075%
50	18.745	2692	2696	2704	rVB	147442	252695	3.77%	0.271%
51	18.868	2711	2717	2722	rBV	4130288	5455527	81.47%	5.845%
52	18.933	2724	2728	2732	rVB3	108834	150293	2.24%	0.161%
53	18.968	2732	2734	2738	rVB2	75520	81791	1.22%	0.088%
54	19.027	2739	2744	2748	rBV2	391999	551624	8.24%	0.591%
55	19.233	2770	2779	2787	rBV	3318242	5406193	80.73%	5.792%
56	19.310	2788	2792	2800	rVB2	145354	272337	4.07%	0.292%
57	19.421	2807	2811	2812	rBV	201365	226266	3.38%	0.242%
58	19.451	2812	2816	2821	rVV	5117936	6388478	95.40%	6.845%
59	19.568	2831	2836	2842	rVB3	156007	356356	5.32%	0.382%
60	19.704	2855	2859	2860	rBV3	143924	190111	2.84%	0.204%
61	19.739	2862	2865	2872	rVB	393787	572913	8.56%	0.614%
62	19.839	2879	2882	2886	rBV	368389	427495	6.38%	0.458%
63	19.898	2887	2892	2896	rVV2	288702	484101	7.23%	0.519%
64	19.933	2896	2898	2903	rVB	114513	150625	2.25%	0.161%
65	20.039	2913	2916	2919	rVB	143783	165897	2.48%	0.178%
66	20.086	2920	2924	2927	rBV2	172292	255033	3.81%	0.273%
67	20.121	2928	2930	2934	rVB	166864	172404	2.57%	0.185%
68	20.498	2990	2994	2999	rVB	291870	399407	5.96%	0.428%
69	20.615	3011	3014	3017	rBV	216790	297654	4.44%	0.319%
70	20.656	3018	3021	3025	rVV2	328194	432225	6.45%	0.463%
71	20.698	3025	3028	3031	rVB	262247	251335	3.75%	0.269%
72	20.756	3031	3038	3042	rBV4	650254	1178578	17.60%	1.263%
73	20.874	3055	3058	3062	rBV	415031	505586	7.55%	0.542%
74	21.027	3072	3084	3088	rBV2	3082978	6696702	100.00%	7.175%
75	21.068	3088	3091	3102	rVB	1544780	2077075	31.02%	2.225%
76	21.192	3109	3112	3116	rVB	250484	295835	4.42%	0.317%

LSC Area Percent Report

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Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	22.886	3394	3400	3406	rBV	916344	2364275	35.31%	2.533%
78	22.998	3414	3419	3426	rVB	558343	932896	13.93%	0.999%
79	23.480	3496	3501	3513	rVB	523972	1262331	18.85%	1.352%
80	23.597	3516	3521	3534	rVB	742342	1636541	24.44%	1.753%
81	23.727	3537	3543	3550	rBV	1348786	2908648	43.43%	3.116%
82	24.686	3701	3706	3717	rVB	442253	1061063	15.84%	1.137%

Sum of corrected areas: 93337339

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
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Misc :
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Instrument :
BNA_M
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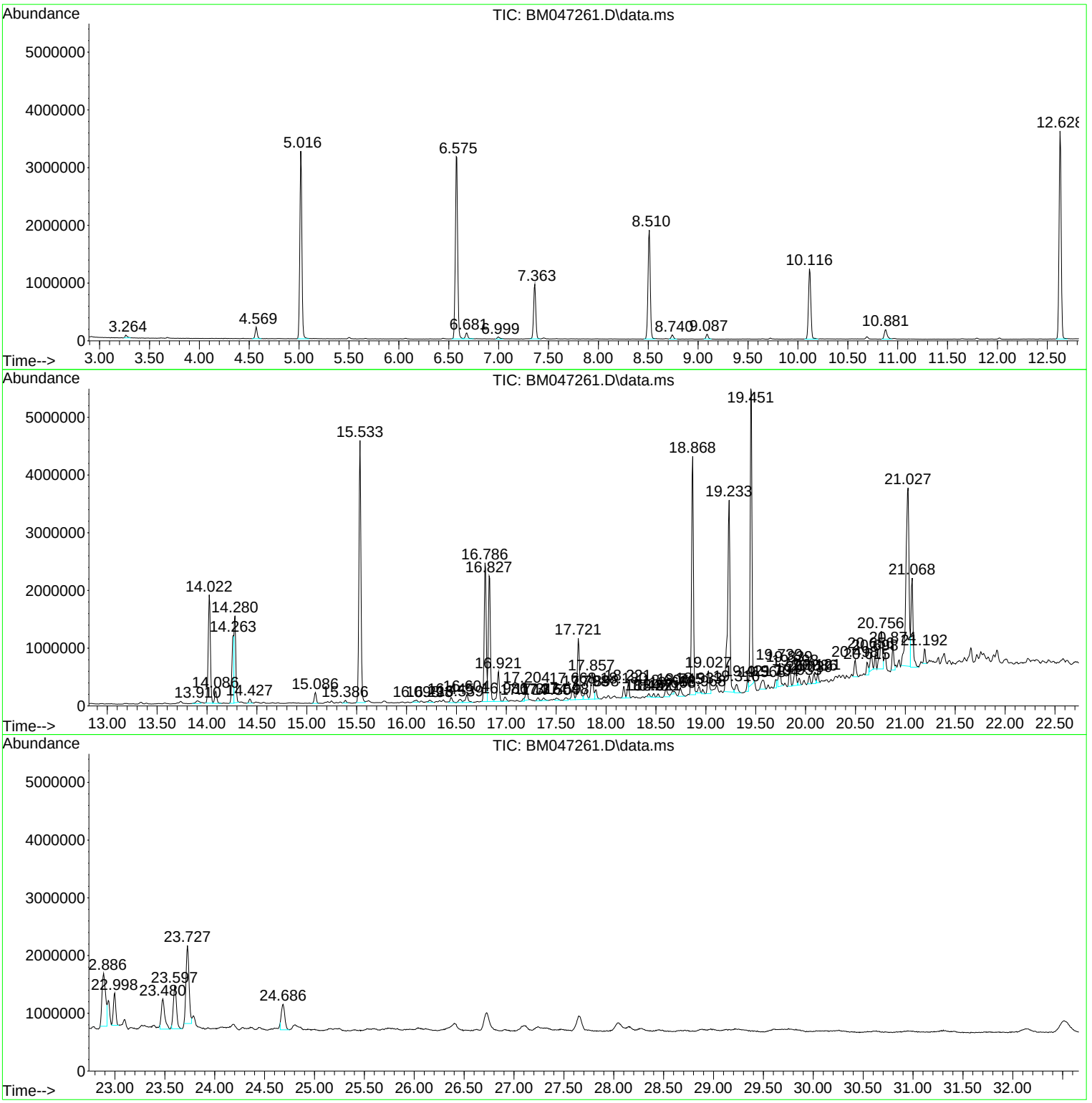
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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\BM081924\
Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

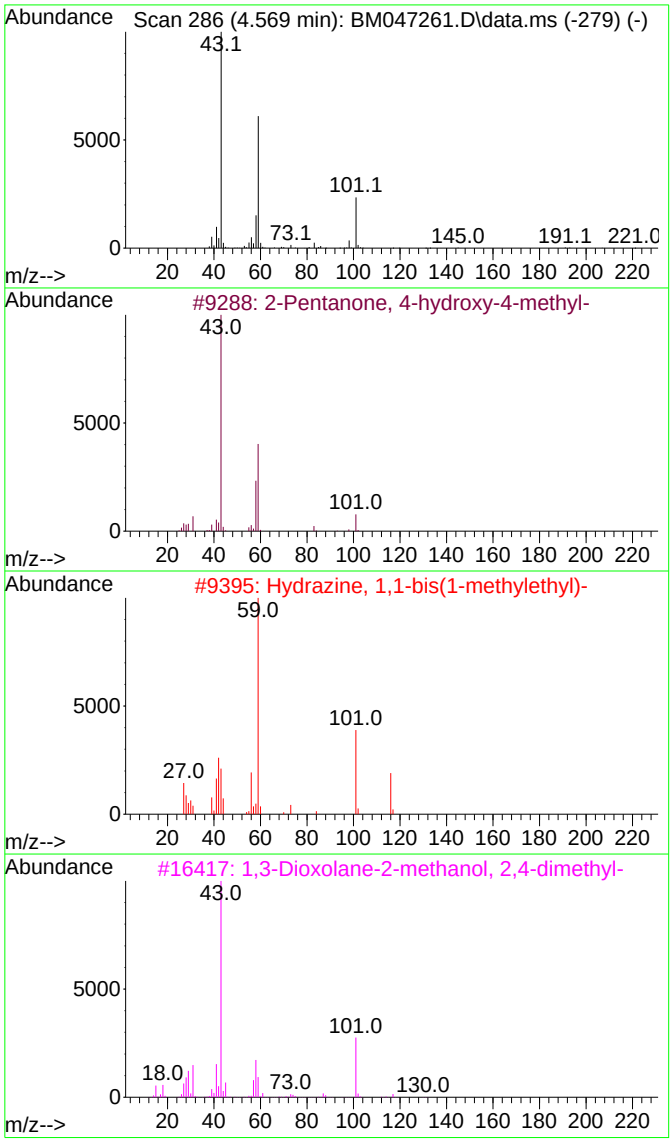
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

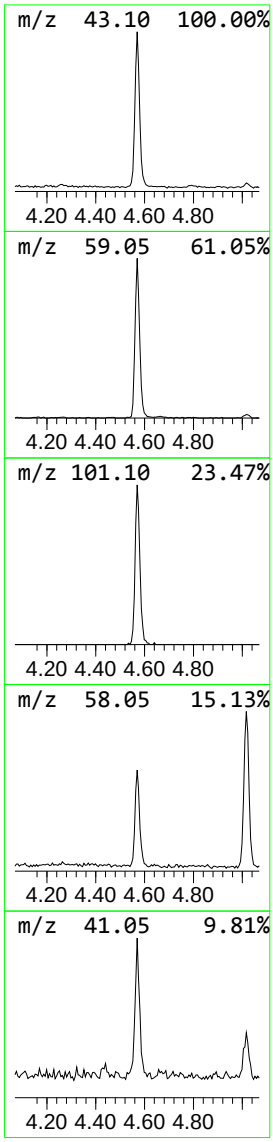
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.87 ng	283180	1,4-Dichlorobenzene-d4	7.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

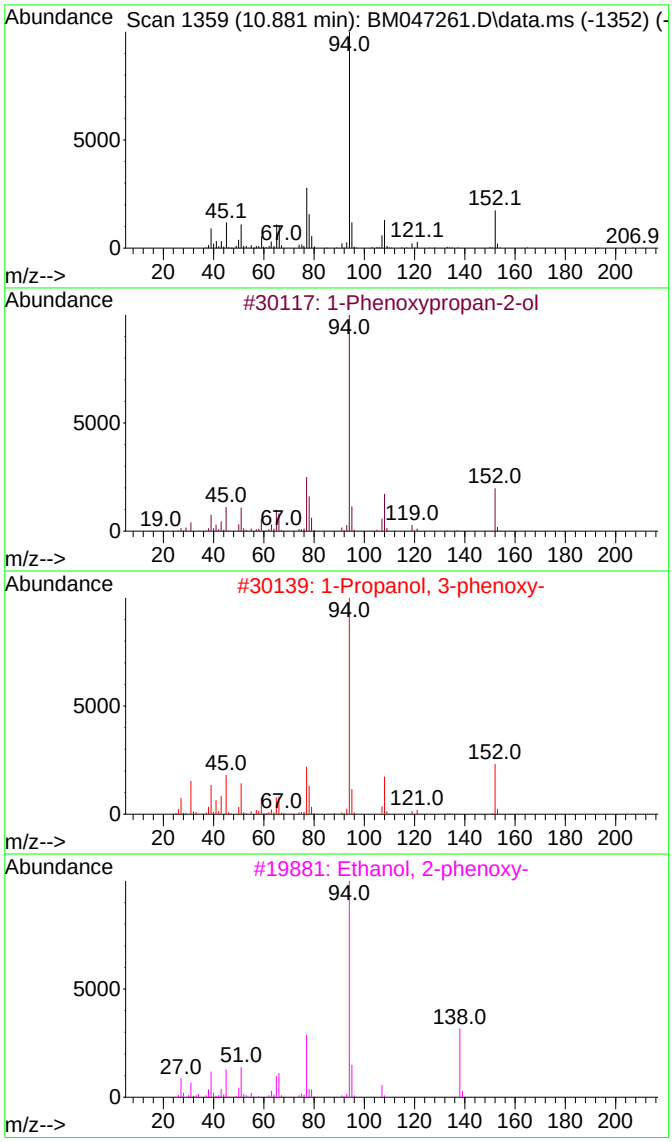
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

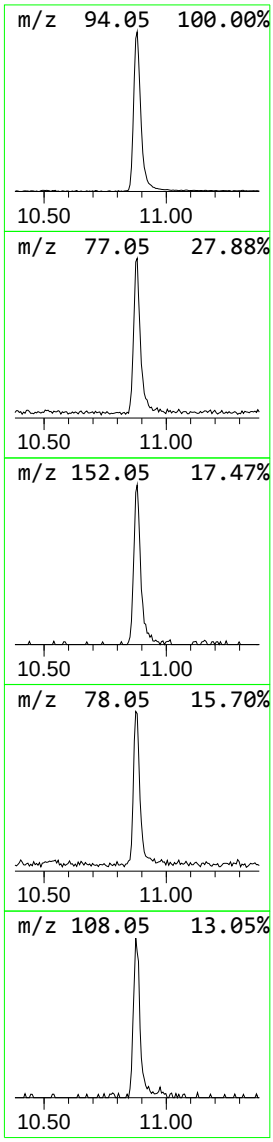
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	3.20 ng	323260	Naphthalene-d8	10.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

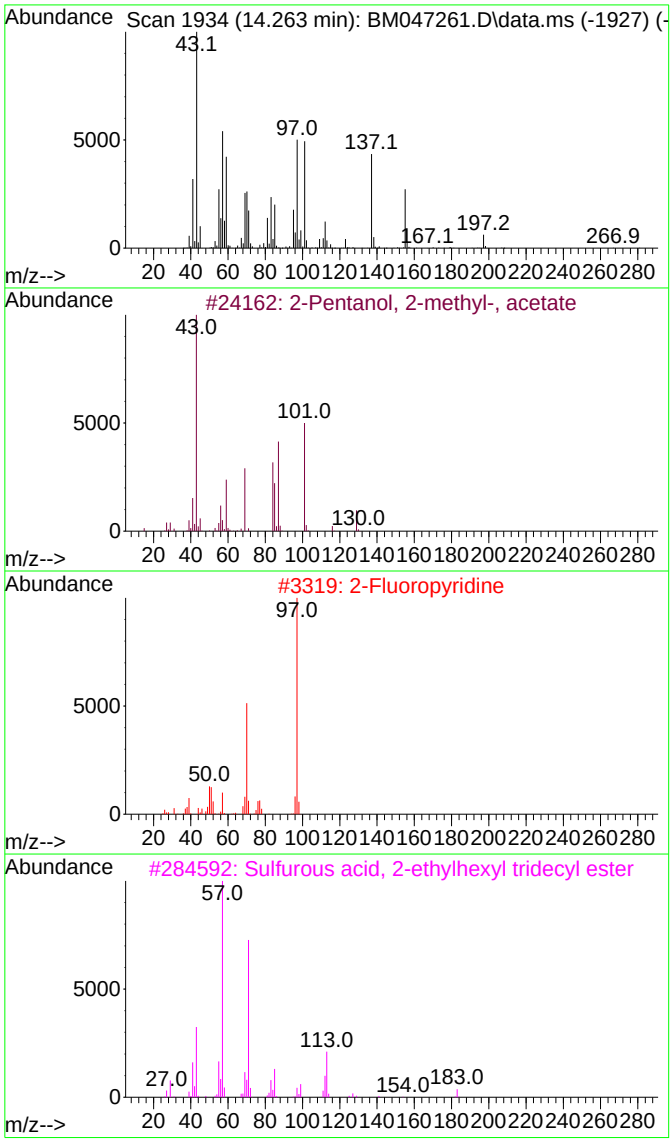
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

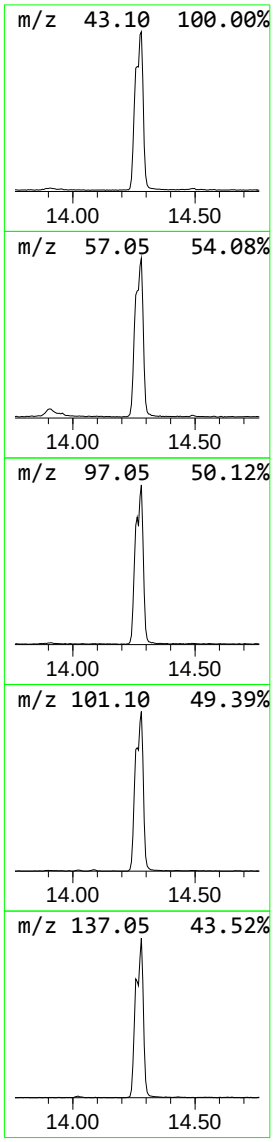
****

Peak Number 4 unknown14.263 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	12.23 ng	1689610	Acenaphthene-d10	14.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
2	2-Fluoropyridine	97	C5H4FN	000372-48-5	10
3	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	10
4	2-(Diethylamino)acetonitrile	112	C6H12N2	003010-02-4	10
5	1-(2-Furyl)-3-buten-1-ol	138	C8H10O2	1000311-94-9	10





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

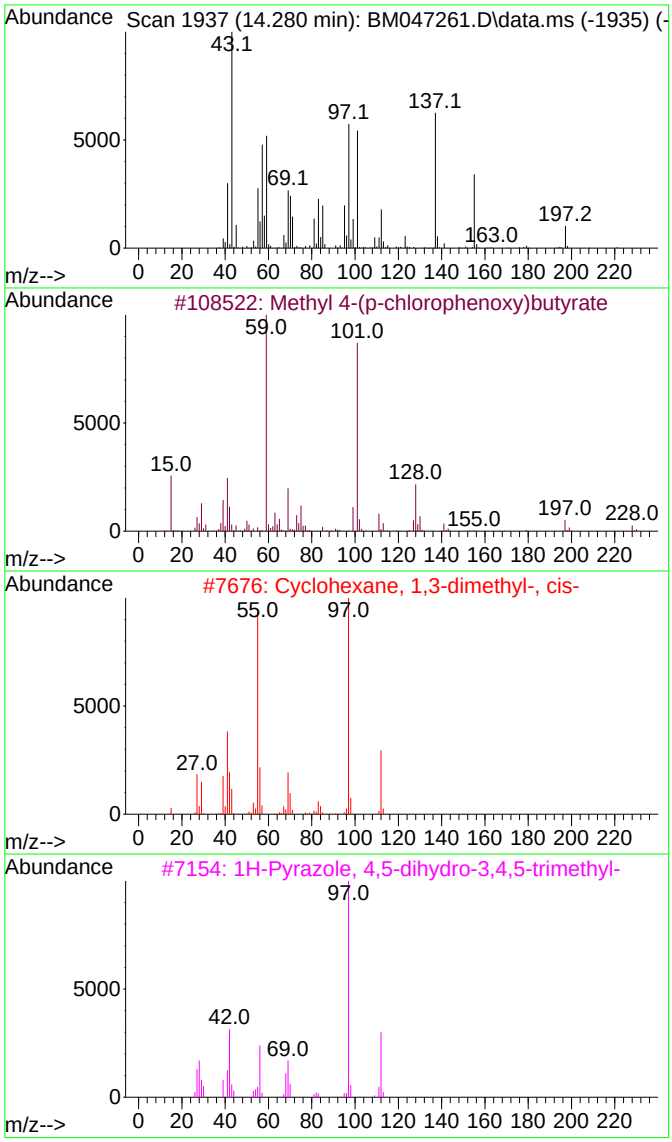
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

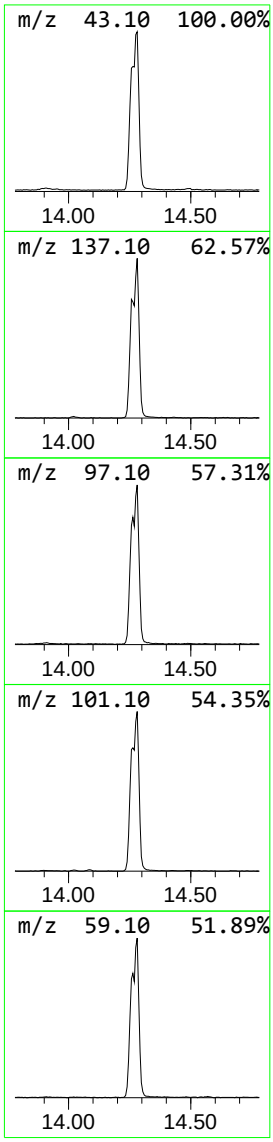
****

Peak Number 5 unknown14.280 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	11.86 ng	1638210	Acenaphthene-d10	14.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 4-(p-chlorophenoxy)butyrate	228	C11H13ClO3	209052-80-2	22
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11
3	1H-Pyrazole, 4,5-dihydro-3,4,5-t...	112	C6H12N2	022591-95-3	10
4	Succinic acid, pent-4-enyl tetra...	382	C23H42O4	1000353-38-0	10
5	Succinic acid, 1-cyclopentylethy...	284	C16H28O4	1000330-20-8	10





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ALS Vial : 18 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

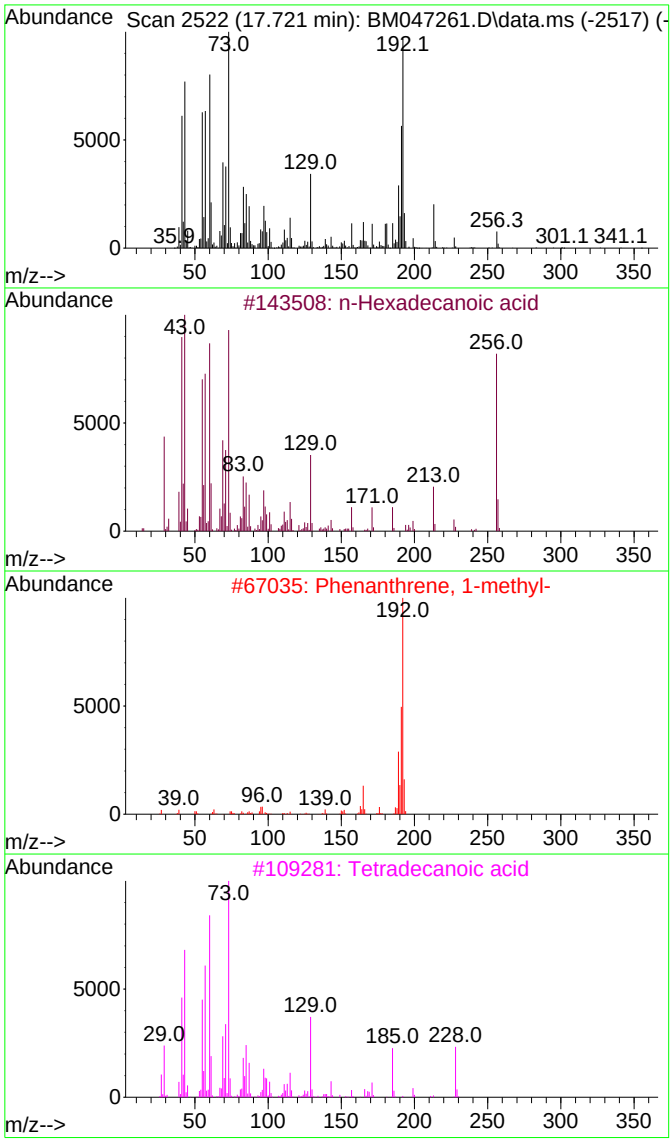
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

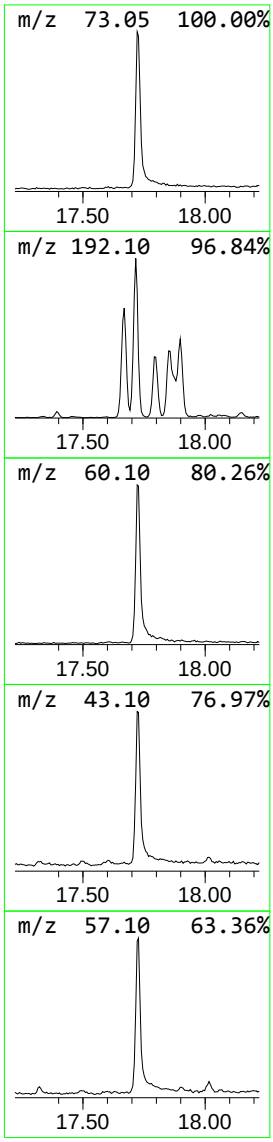
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	9.29 ng	1634110	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

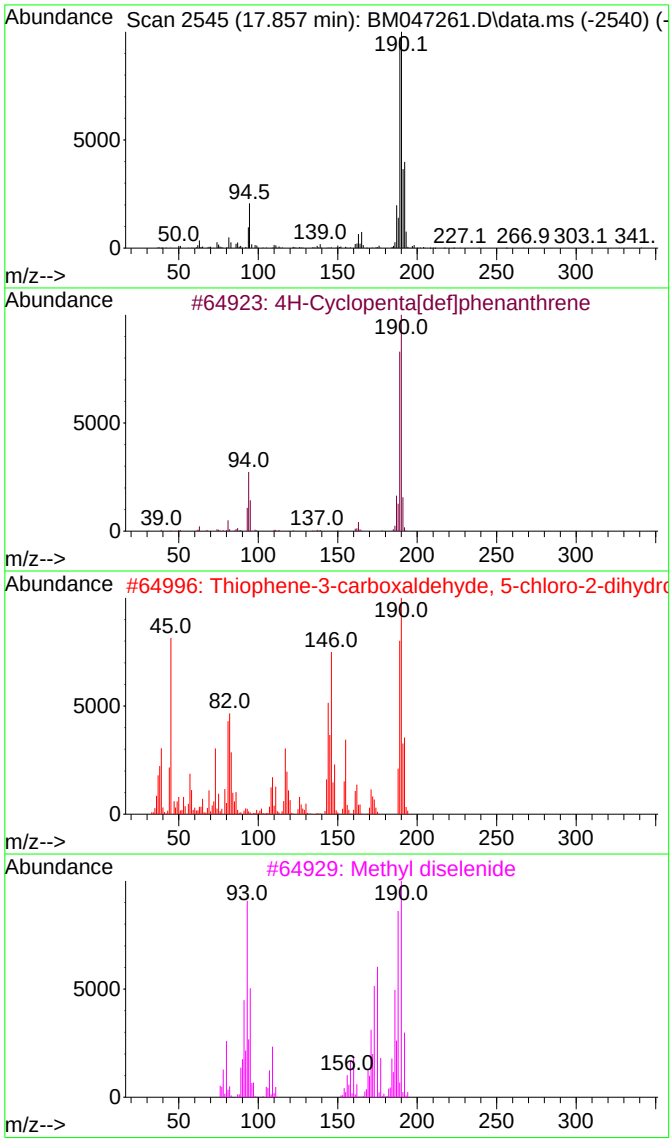
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

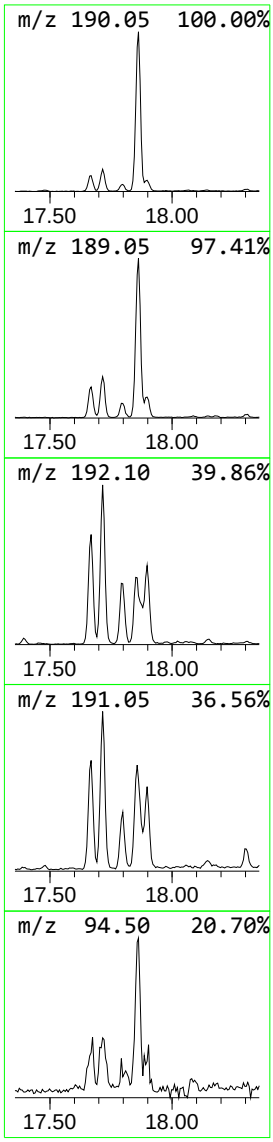
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.857	4.46 ng	784415	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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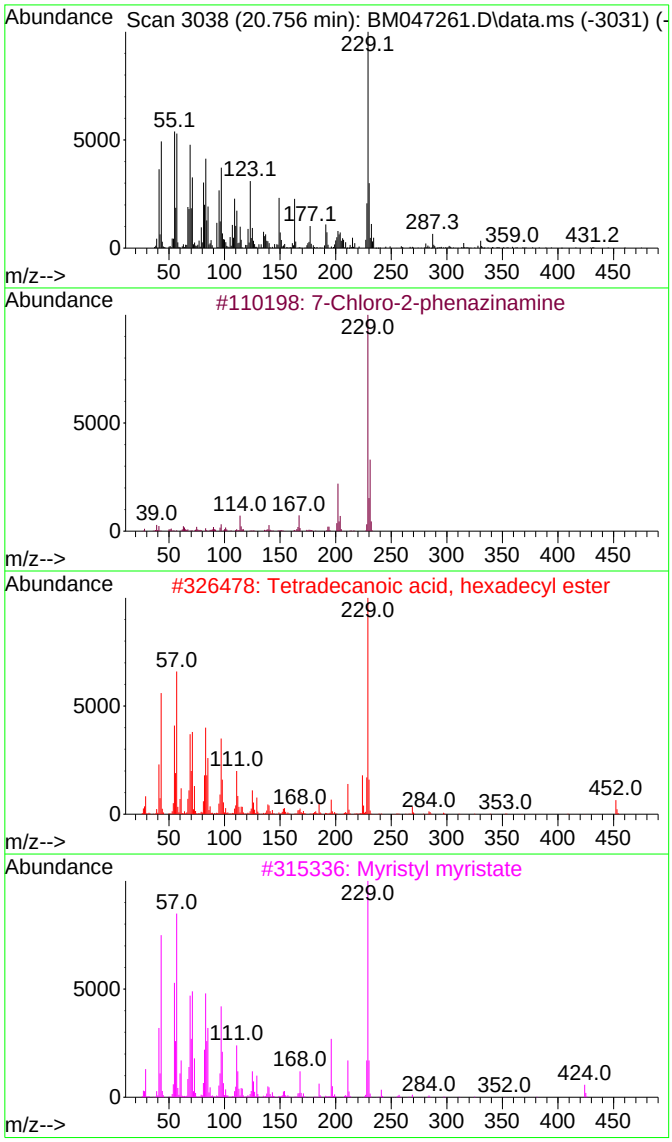
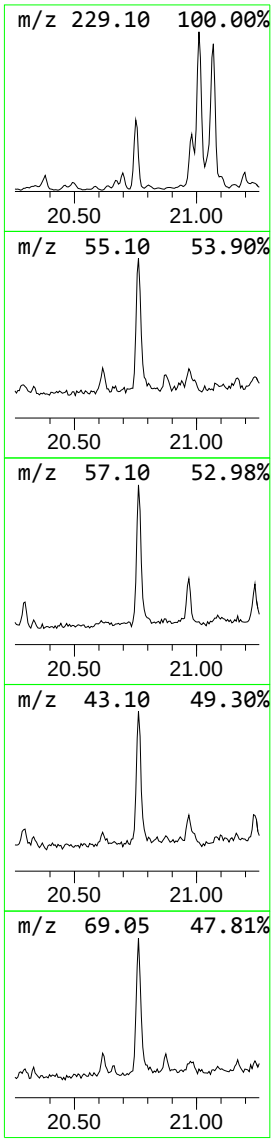
Peak Number 8 unknown20.756 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	3.52 ng	1178580	Chrysene-d12	21.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Chloro-2-phenazinamine	229	C12H8ClN3	023677-11-4	38
2	Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	38
3	Myristyl myristate	424	C28H56O2	003234-85-3	38
4	Benzo(a)acridine	229	C17H11N	000225-11-6	37
5	Benzimidazole-5-amine, 1-methyl-...	229	C12H11N3S	021444-73-5	35





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Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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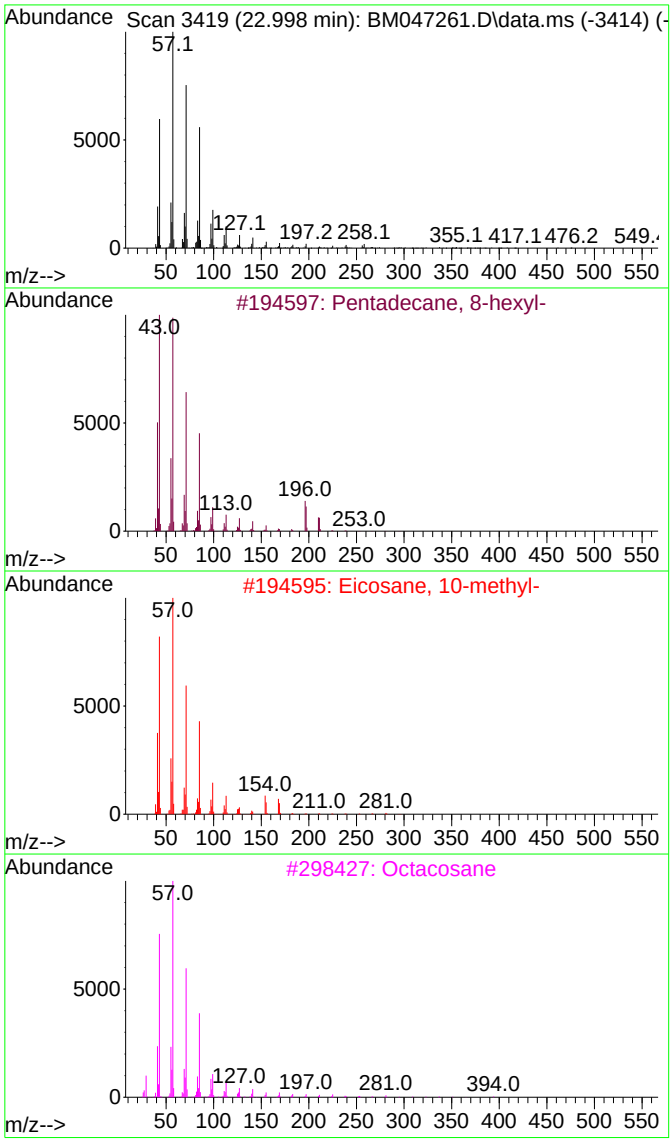
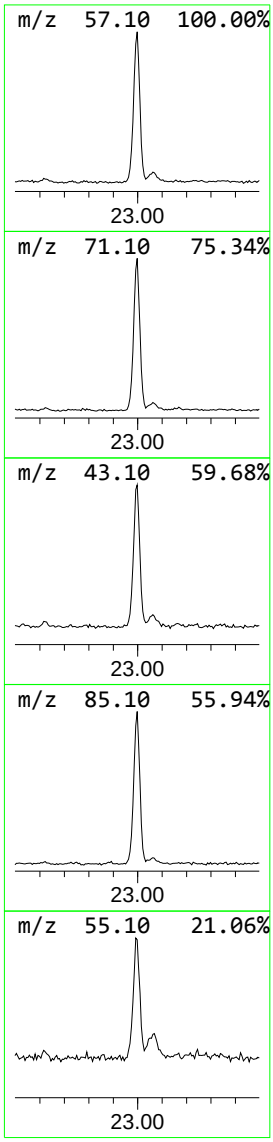
Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.997	6.41 ng	932896	Perylene-d12	23.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Octacosane	394	C28H58	000630-02-4	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Tetracosane	338	C24H50	000646-31-1	90





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Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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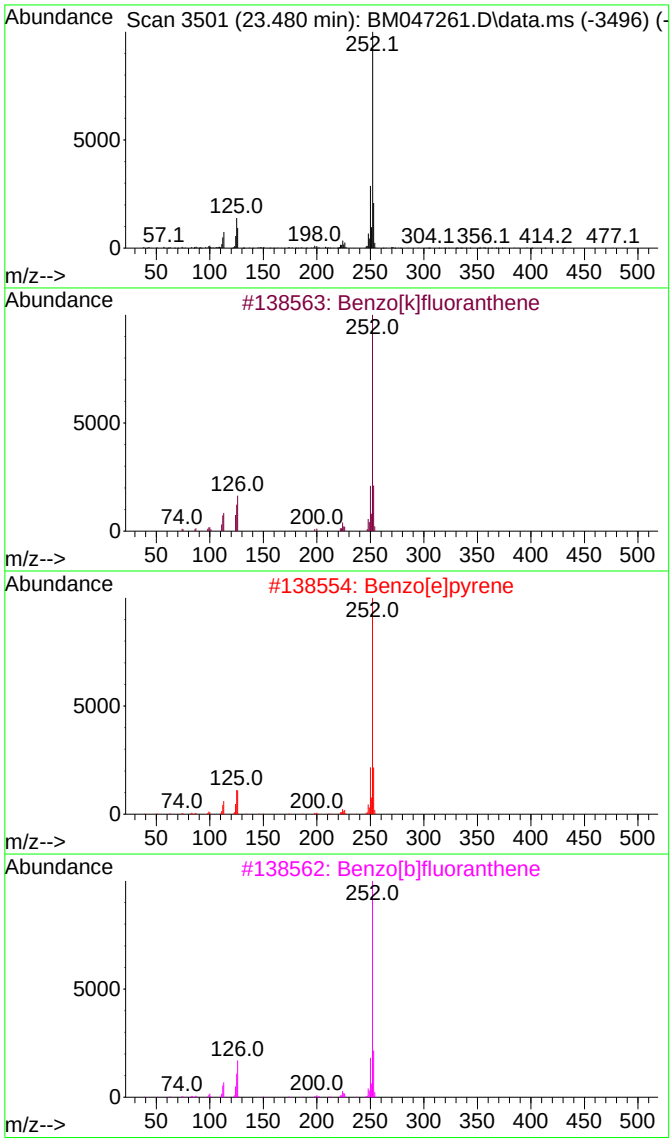
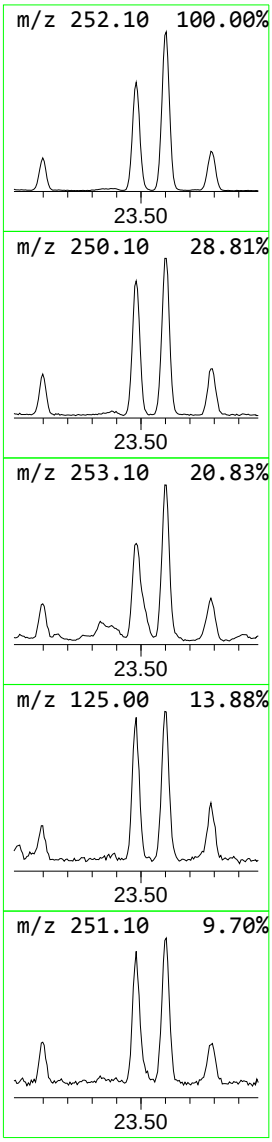
Peak Number 10 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.480	8.68 ng	1262330	Perylene-d12	23.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





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Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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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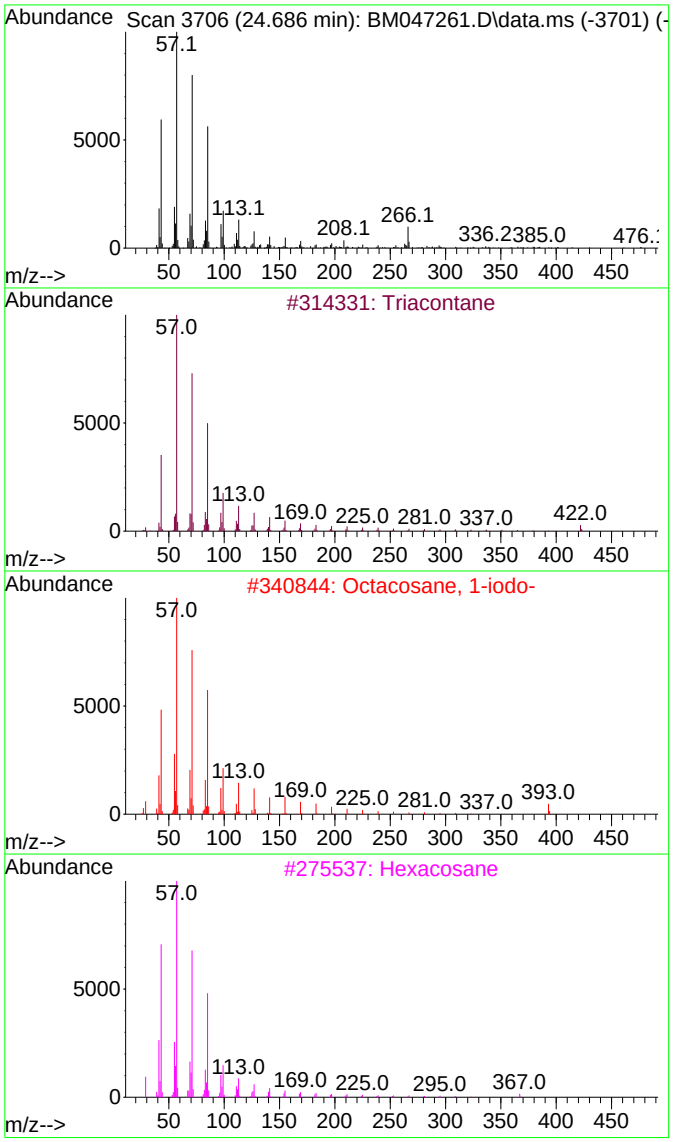
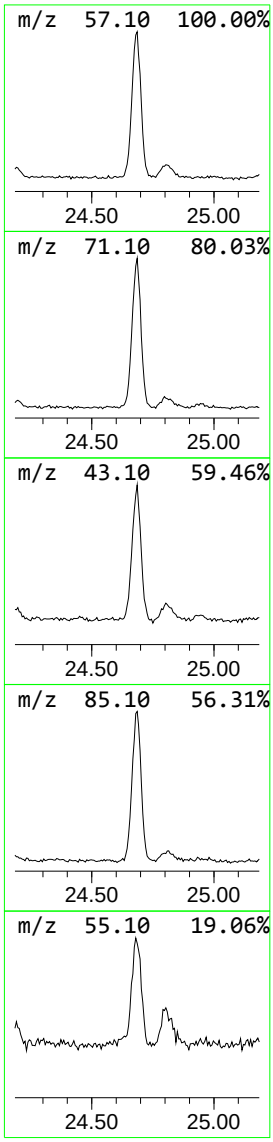
Peak Number 11 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.686	7.30 ng	1061060	Perylene-d12	23.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

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Data File : BM047261.D
Acq On : 19 Aug 2024 20:48
Operator : RC/JU
Sample : P3643-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0-0.5-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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-...	4.569	3.9	ng	283180	1	7.363	1461830	20.0
1-Phenoxypropan...	10.881	3.2	ng	323260	2	10.116	2017790	20.0
unknown14.263	14.263	12.2	ng	1689610	3	14.022	2763520	20.0
unknown14.280	14.280	11.9	ng	1638210	3	14.022	2763520	20.0
n-Hexadecanoic ...	17.721	9.3	ng	1634110	4	16.786	3517990	20.0
4H-Cyclopenta[d...	17.857	4.5	ng	784415	4	16.786	3517990	20.0
unknown20.756	20.756	3.5	ng	1178580	5	21.027	6696700	20.0
Pentadecane, 8-...	22.997	6.4	ng	932896	6	23.727	2908650	20.0
Benzo[e]pyrene	23.480	8.7	ng	1262330	6	23.727	2908650	20.0
Triacontane	24.686	7.3	ng	1061060	6	23.727	2908650	20.0