LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028597.D
Acq On : 28 Jan 2021 20:58
Operator : CG/JU
Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SIDEWALK

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.028	139	143	151	rVB	5543	8369	1.12%	0.116%
2	5.510	389	395	411	rVB	202965	312956	41.96%	4.337%
3	7.151	668	674	684	rBV	195762	334114	44.80%	4.630%
4	7.963	806	812	819	rVB	141068	217951	29.23%	3.020%
5	9.140	1005	1012	1018	rBV	125870	205004	27.49%	2.841%
6	10.781	1284	1291	1296	rBV	170982	282882	37.93%	3.920%
7	11.781	1456	1461	1466	rVB3	5304	8346	1.12%	0.116%
8	12.433	1567	1572	1577	rVB3	5100	7960	1.07%	0.110%
9	12.563	1588	1594	1606	rBV2	8032	18304	2.45%	0.254%
10	13.233	1702	1708	1716	rVB	271698	386395	51.81%	5.354%
11	13.927	1821	1826	1832	rBV2	4047	7802	1.05%	0.108%
12	14.069	1846	1850	1857	rVB2	10865	17971	2.41%	0.249%
13	14.245	1877	1880	1890	rVB3	6238	12638	1.69%	0.175%
14	14.333	1890	1895	1903	rBV	18168	30440	4.08%	0.422%
15	14.492	1919	1922	1928	rVB2	6383	8578	1.15%	0.119%
16	14.610	1931	1942	1949	rBV	230455	345602	46.34%	4.789%
17	15.016	2005	2011	2016	rBV6	6428	11831	1.59%	0.164%
18	15.222	2041	2046	2052	rBV5	3556	7792	1.04%	0.108%
19	15.392	2071	2075	2079	rBV3	5275	8047	1.08%	0.112%
20	15.439	2079	2083	2087	rVB4	5903	8100	1.09%	0.112%
21	15.651	2114	2119	2122	rBV3	4204	8056	1.08%	0.112%
22	16.098	2189	2195	2207	rVB	198060	281757	37.78%	3.904%
23	16.304	2225	2230	2231	rBV2	9549	12870	1.73%	0.178%
24	16.321	2231	2233	2239	rVB5	11773	16920	2.27%	0.234%
25	16.427	2247	2251	2254	rBV	7723	11234	1.51%	0.156%
26	16.486	2258	2261	2267	rVV2	5839	10516	1.41%	0.146%
27	16.545	2268	2271	2277	rVB3	5724	8041	1.08%	0.111%
28	16.663	2283	2291	2293	rBV6	5838	13753	1.84%	0.191%
29	16.686	2293	2295	2300	rVV5	7687	11274	1.51%	0.156%
30	16.739	2300	2304	2311	rVB6	12197	21359	2.86%	0.296%
31	16.810	2311	2316	2319	rBV	9732	13315	1.79%	0.185%
32	16.874	2324	2327	2331	rVV3	6811	8788	1.18%	0.122%
33	17.004	2345	2349	2354	rBV3	5390	9126	1.22%	0.126%
34	17.092	2359	2364	2368	rVV5	13676	20350	2.73%	0.282%
35	17.239	2384	2389	2396	rVB6	6327	15032	2.02%	0.208%
36	17.345	2401	2407	2411	rBV	253505	368459	49.41%	5.106%

LSC Area Percent Report

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Acq On : 28 Jan 2021 20:58
Operator : CG/JU
Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SIDEWALK

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.386	2411	2414	2421	rVB	62086	81013	10.86%	1.123%
38	17.474	2424	2429	2434	rBV	38843	61032	8.18%	0.846%
39	17.621	2450	2454	2457	rBV5	7356	11154	1.50%	0.155%
40	17.745	2472	2475	2480	rBV	7853	10161	1.36%	0.141%
41	17.815	2484	2487	2492	rVB5	7888	10329	1.39%	0.143%
42	18.221	2550	2556	2560	rBV2	213994	311520	41.77%	4.317%
43	18.404	2582	2587	2591	rBV4	21220	40621	5.45%	0.563%
44	18.510	2601	2605	2609	rBV4	12658	22336	3.00%	0.310%
45	18.598	2617	2620	2626	rVB7	7578	11487	1.54%	0.159%
46	18.710	2632	2639	2643	rBV4	21297	37839	5.07%	0.524%
47	18.757	2643	2647	2652	rVB4	11946	18952	2.54%	0.263%
48	18.968	2678	2683	2687	rBV	39604	53411	7.16%	0.740%
49	19.127	2705	2710	2714	rBV3	26160	50462	6.77%	0.699%
50	19.351	2742	2748	2749	rBV2	158214	214974	28.83%	2.979%
51	19.380	2749	2753	2763	rVB2	389295	745768	100.00%	10.334%
52	19.492	2768	2772	2777	rVB	128410	162902	21.84%	2.257%
53	19.745	2811	2815	2823	rVB2	144133	227052	30.45%	3.146%
54	19.845	2829	2832	2839	rVB2	29098	44631	5.98%	0.618%
55	19.939	2843	2848	2853	rBV	364066	426076	57.13%	5.904%
56	20.809	2993	2996	2999	rBV	48306	58213	7.81%	0.807%
57	21.180	3055	3059	3062	rBV2	74929	97233	13.04%	1.347%
58	21.386	3091	3094	3097	rVB	43020	44209	5.93%	0.613%
59	21.486	3104	3111	3114	rBV2	350035	573506	76.90%	7.947%
60	21.515	3114	3116	3125	rVB	103799	139554	18.71%	1.934%
61	23.068	3376	3380	3385	rBV	95403	184310	24.71%	2.554%
62	23.650	3475	3479	3487	rVB	92028	159613	21.40%	2.212%
63	23.750	3491	3496	3502	rVB2	199413	346411	46.45%	4.800%

Sum of corrected areas: 7216701

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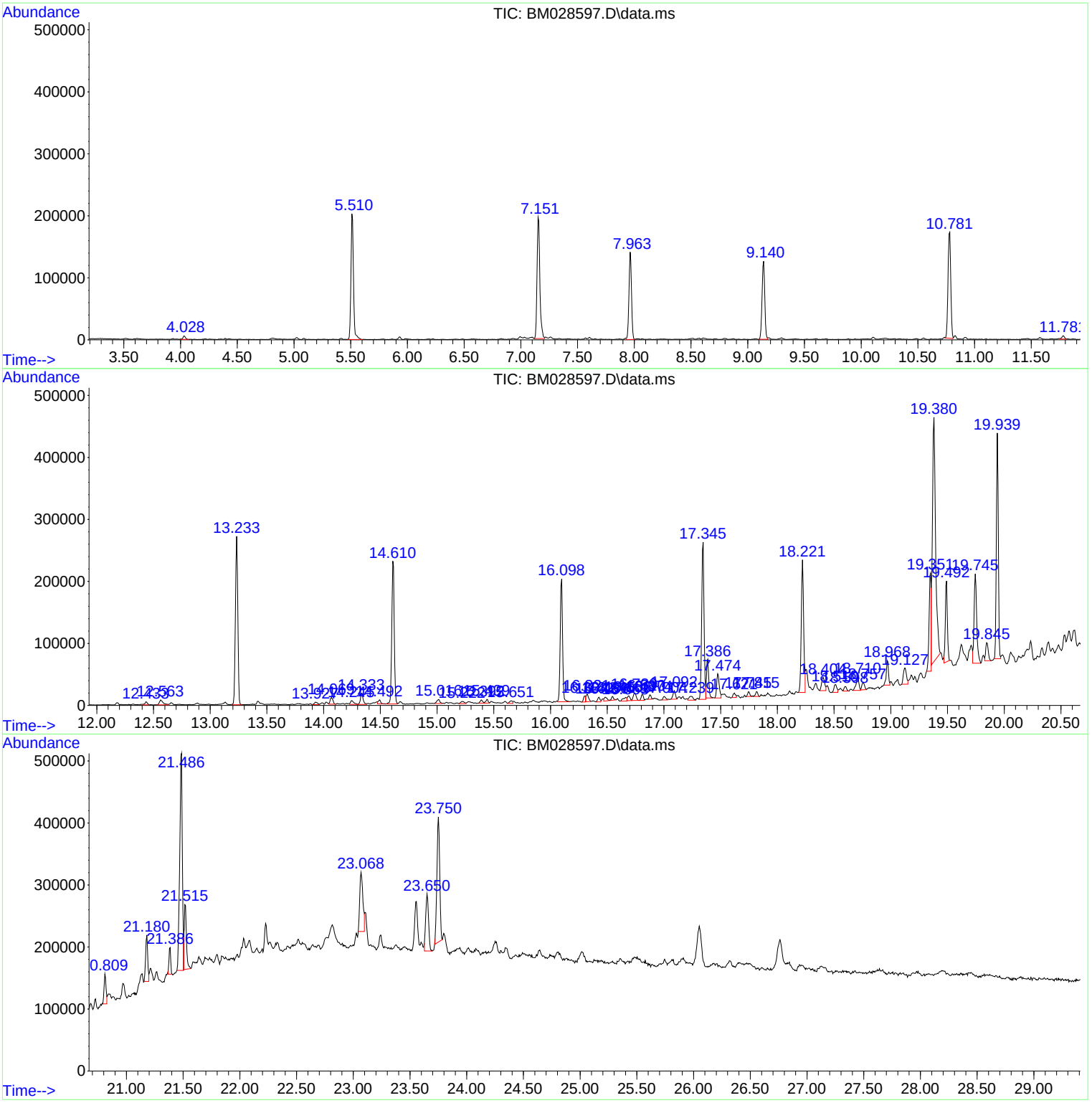
Instrument :
BNA_M
ClientSampleId :
SIDEWALK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BM028597.D
Acq On : 28 Jan 2021 20:58
Operator : CG/JU
Sample : M1256-02 2X
Misc :
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Instrument : BNA_M
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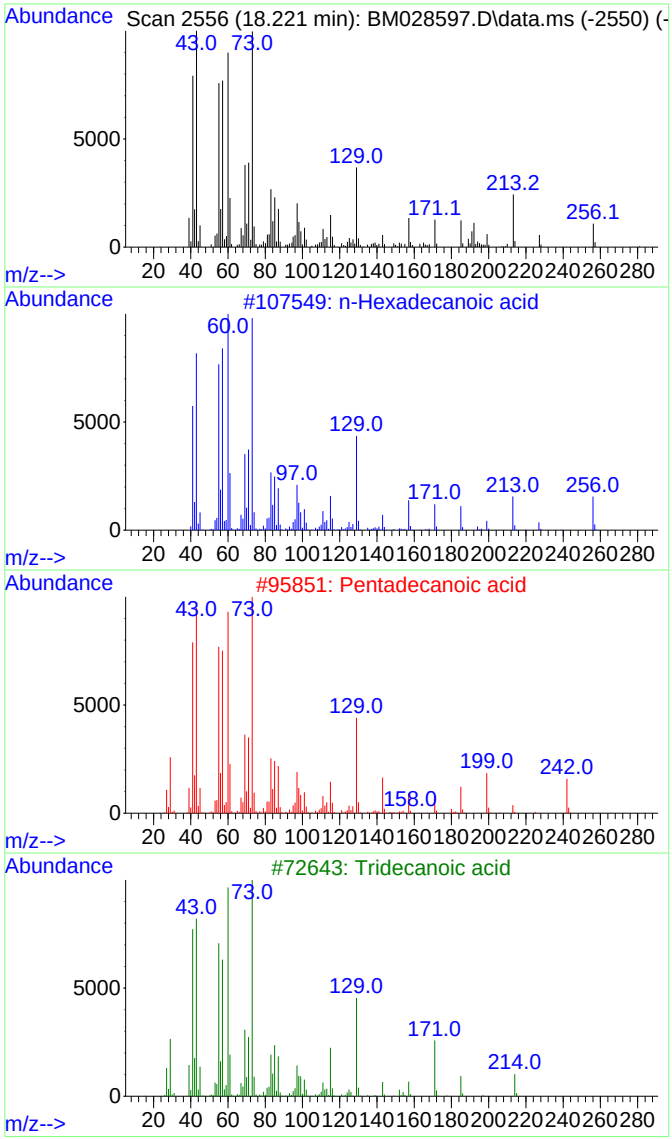
TIC Integration Parameters: LSCINT.P

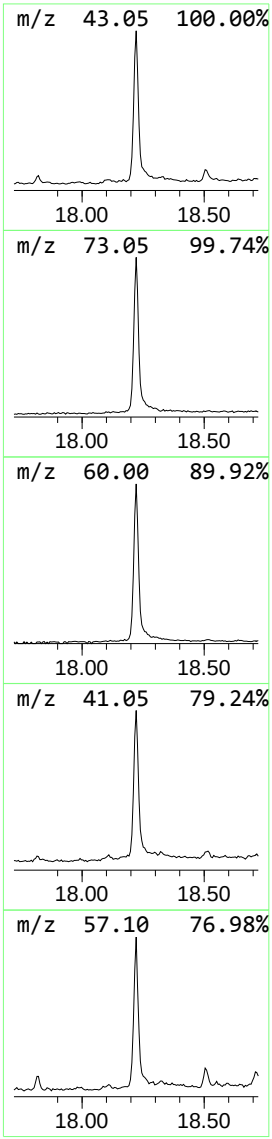
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	16.91 ng	311520	Phenanthrene-d10	17.345

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028597.D
Acq On : 28 Jan 2021 20:58
Operator : CG/JU
Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SIDEWALK

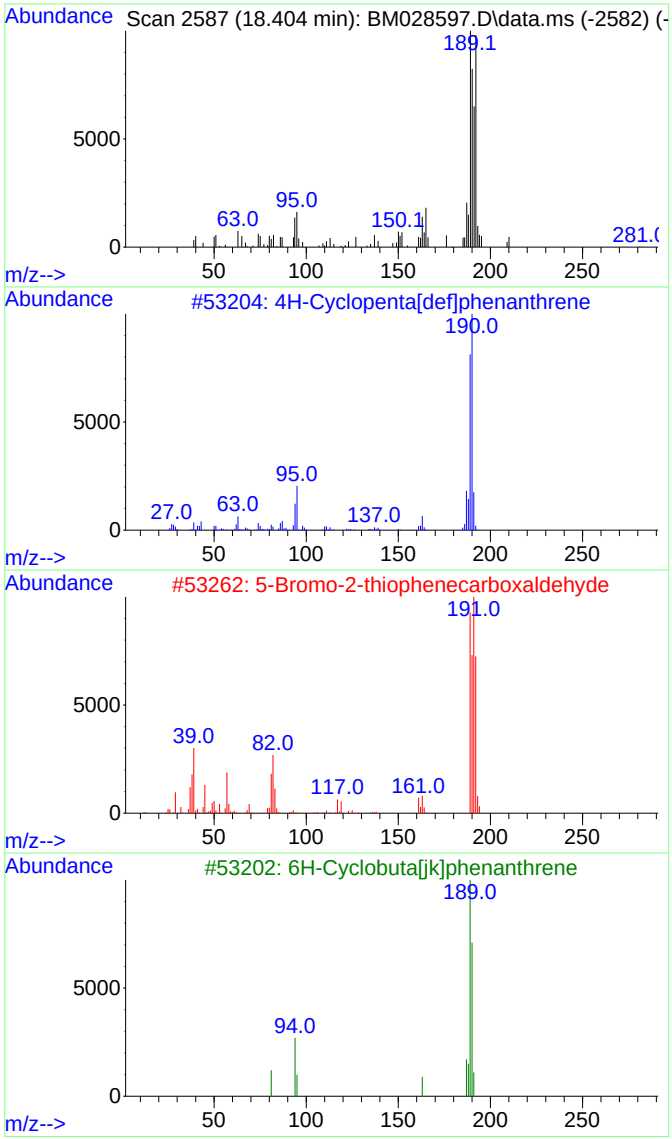
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

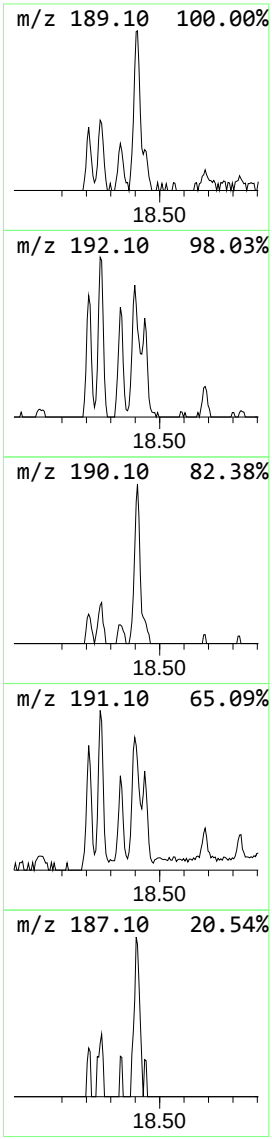
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.404	2.20 ng	40621	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	59
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
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Operator : CG/JU
Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SIDEWALK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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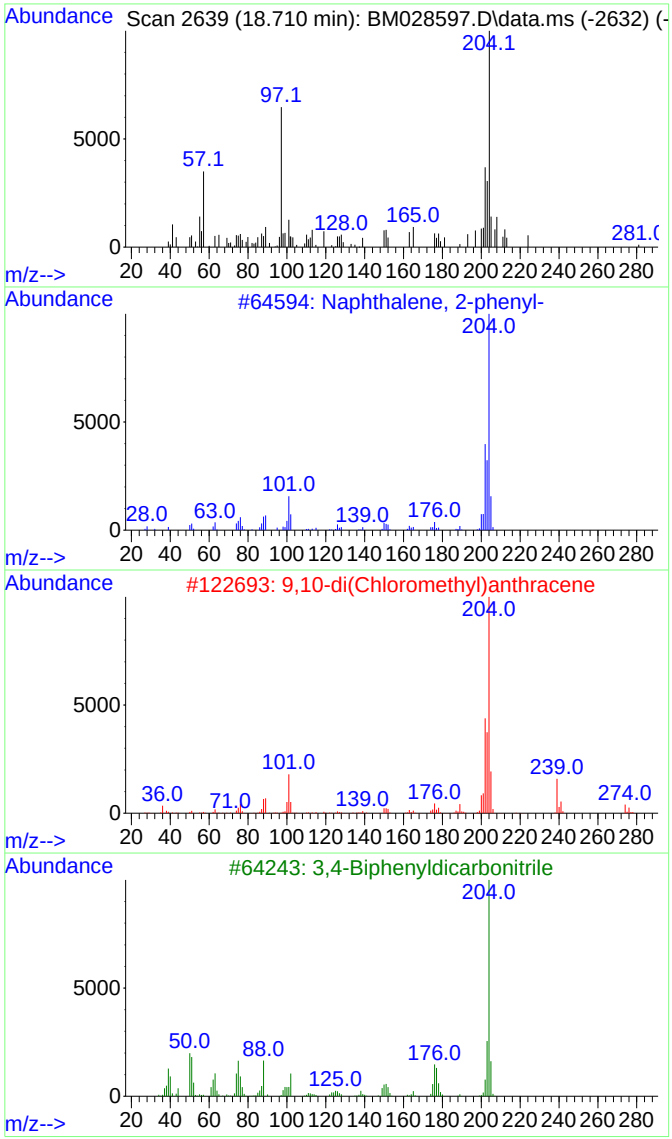
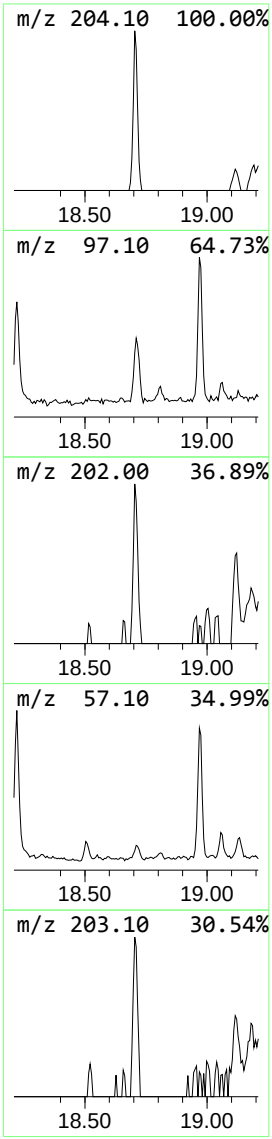
Peak Number 3 Naphthalene, 2-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.709	2.05 ng	37839	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	55
2	9,10-di(Chloromethyl)anthracene	274	C16H12Cl2	010387-13-0	52
3	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	49
4	2-Hexenoic acid, 4-methylphenyl ...	204	C13H16O2	069687-91-8	47
5	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	47





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Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SIDEWALK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
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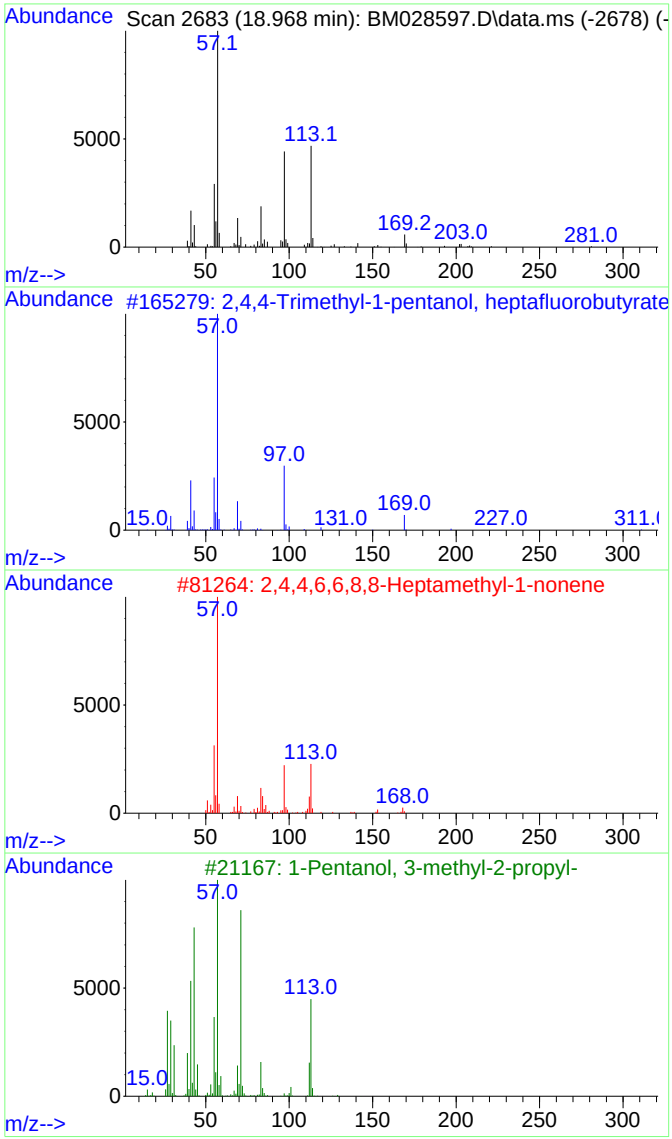
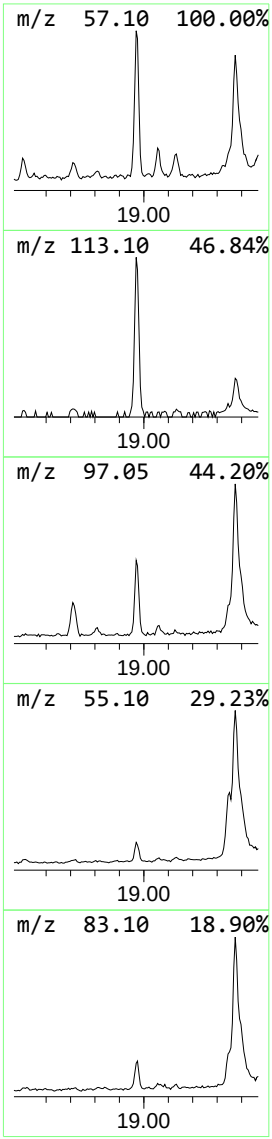
Peak Number 4 unknown18.968 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.968	2.90 ng	53411	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	43
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	40
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32





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Misc :
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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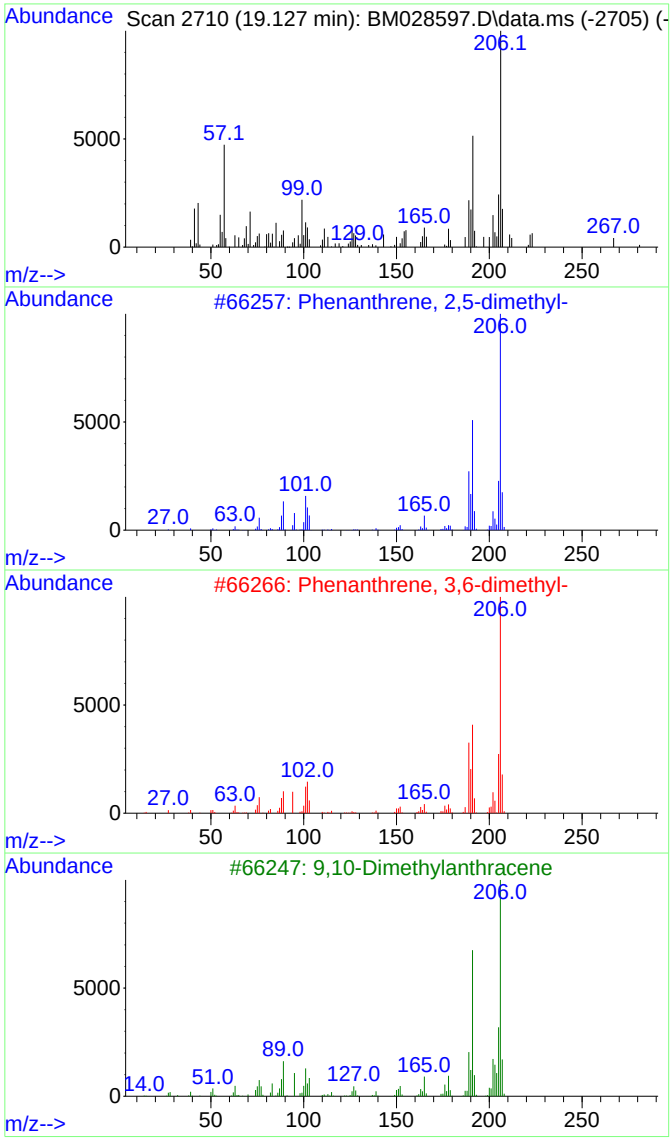
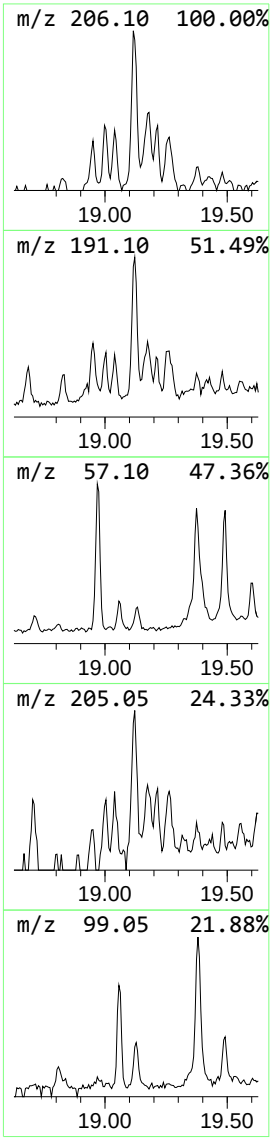
****
Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.127	2.74 ng	50462	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	86
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	81
4	Phenanthrene, 4,5-dimethyl-	206	C16H14	003674-69-9	76
5	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	76





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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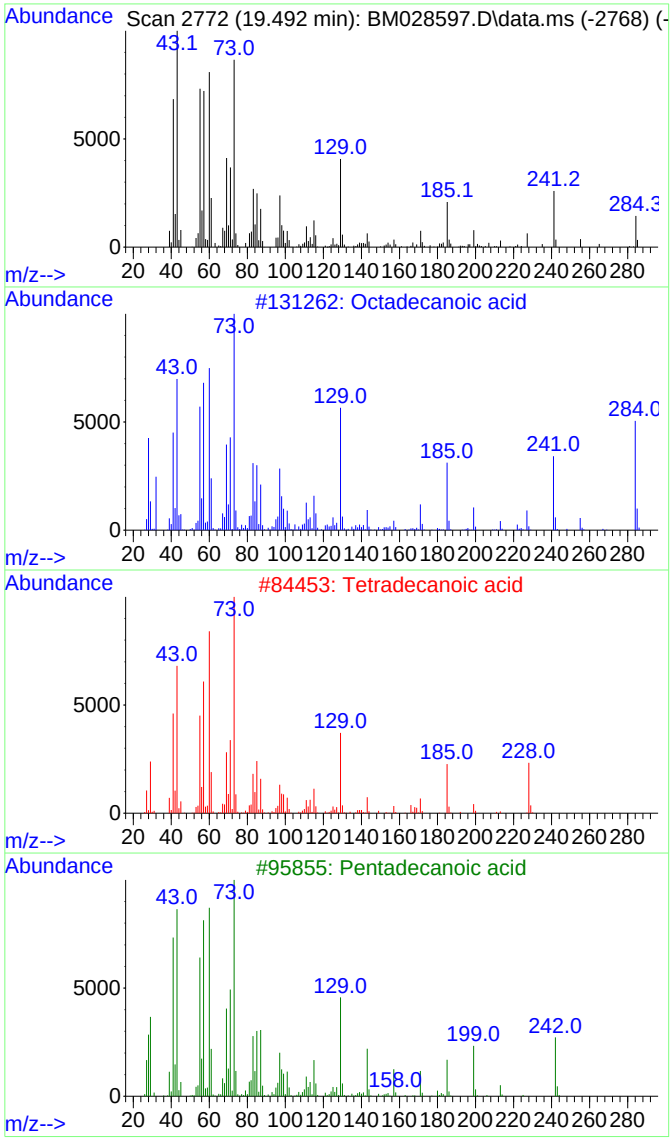
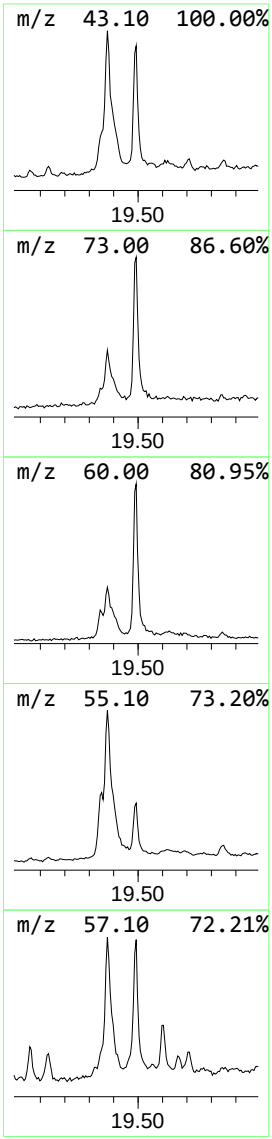
Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	5.68 ng	162902	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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Operator : CG/JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SIDEWALK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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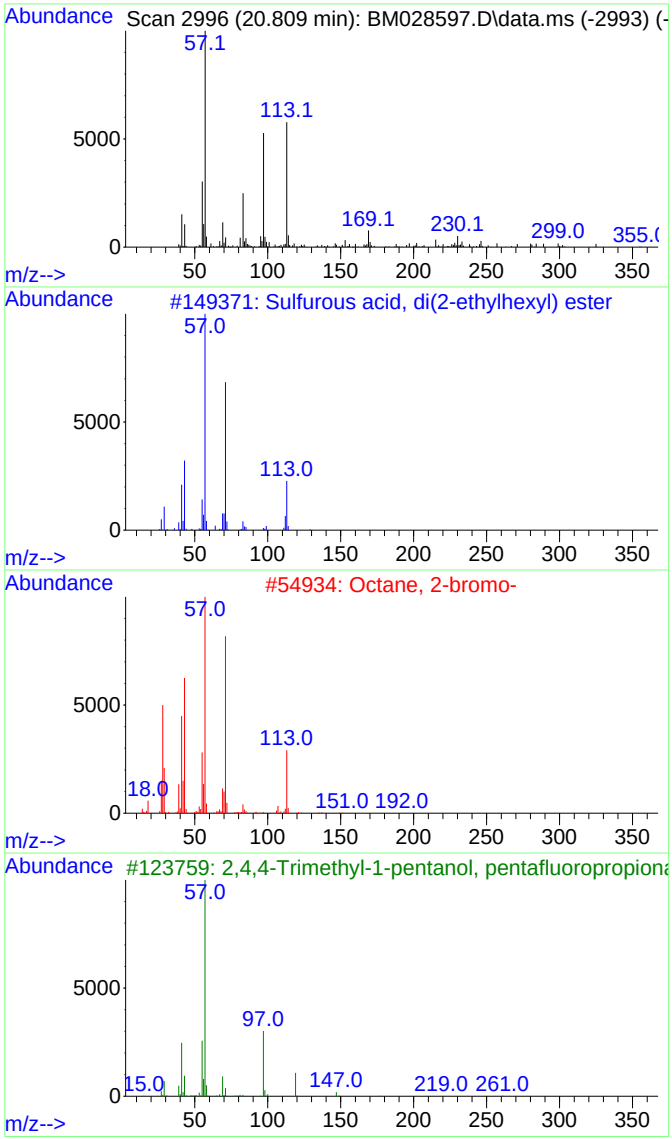
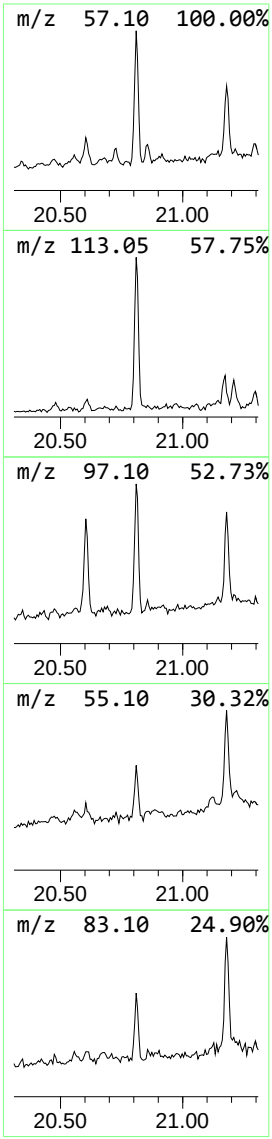
Peak Number 7 unknown20.809 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	2.03 ng	58213	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	35
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27
4	Piperazine, 1-methyl-4-(2-phenox...	220	C13H20N2O	328002-65-9	18
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028597.D
Acq On : 28 Jan 2021 20:58
Operator : CG/JU
Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SIDEWALK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

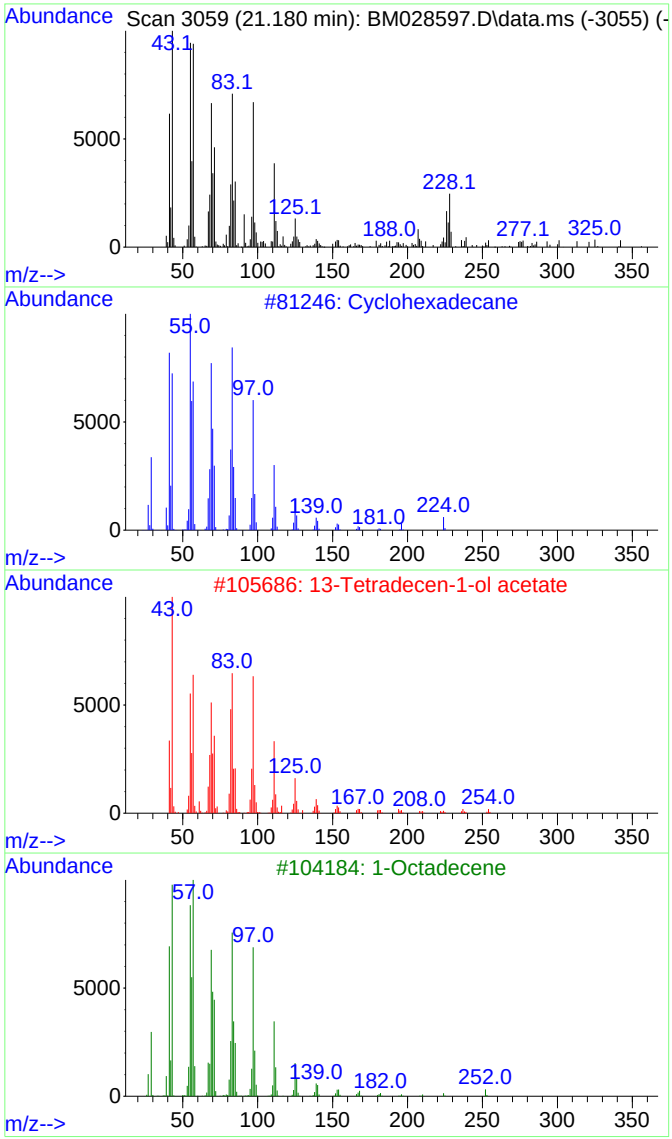
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

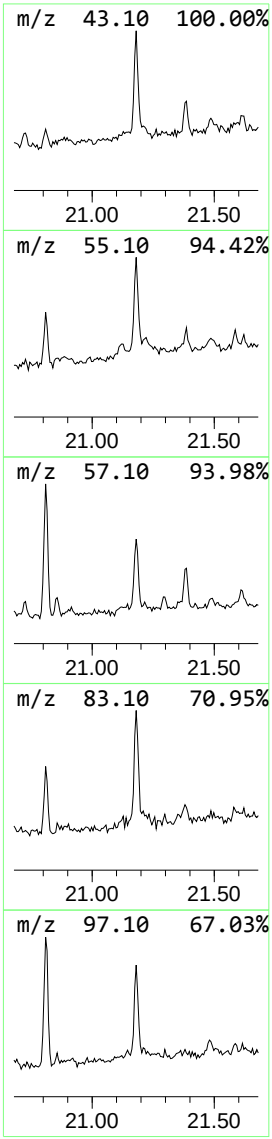
****

Peak Number 8 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	3.39 ng	97233	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	93
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	89
3	1-Octadecene	252	C18H36	000112-88-9	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
Data File : BM028597.D
Acq On : 28 Jan 2021 20:58
Operator : CG/JU
Sample : M1256-02 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SIDEWALK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	16.9	ng	311520	4	17.345	368459	20.0
4H-Cyclopenta[d...	18.404	2.2	ng	40621	4	17.345	368459	20.0
Naphthalene, 2-...	18.709	2.0	ng	37839	4	17.345	368459	20.0
unknown18.968	18.968	2.9	ng	53411	4	17.345	368459	20.0
Phenanthrene, 2...	19.127	2.7	ng	50462	4	17.345	368459	20.0
Octadecanoic acid	19.492	5.7	ng	162902	5	21.486	573506	20.0
unknown20.809	20.809	2.0	ng	58213	5	21.486	573506	20.0
Cyclohexadecane	21.180	3.4	ng	97233	5	21.486	573506	20.0