LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032724\
Data File : BM044795.D
Acq On : 28 Mar 2024 00:47
Operator : MA/JU
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : EXTRA-PILE

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-BM031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044795.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.522	70	74	85	rVB	35139	64629	1.38%	0.114%
2	5.293	368	375	385	rBV	2754924	4003364	85.32%	7.042%
3	6.863	634	642	655	rBV	2603378	4174527	88.96%	7.344%
4	7.681	774	781	788	rBV	810524	1272057	27.11%	2.238%
5	8.845	970	979	993	rBV	1513052	2604787	55.51%	4.582%
6	10.263	1213	1220	1231	rBV3	18185	49751	1.06%	0.088%
7	10.457	1245	1253	1267	rVB	963809	1694066	36.10%	2.980%
8	12.945	1668	1676	1691	rBV	3136925	4692333	100.00%	8.254%
9	13.639	1788	1794	1800	rBV6	24758	53654	1.14%	0.094%
10	13.739	1807	1811	1815	rVB4	40194	58853	1.25%	0.104%
11	14.227	1888	1894	1899	rVB	32737	49120	1.05%	0.086%
12	14.327	1899	1911	1917	rBV	1270583	1922388	40.97%	3.382%
13	14.392	1917	1922	1929	rVB	196920	310323	6.61%	0.546%
14	14.539	1942	1947	1948	rBV	58086	73019	1.56%	0.128%
15	14.733	1975	1980	1990	rVB	66402	110949	2.36%	0.195%
16	15.186	2053	2057	2062	rVB2	36547	50937	1.09%	0.090%
17	15.386	2086	2091	2097	rBV	151864	225051	4.80%	0.396%
18	15.680	2137	2141	2150	rVB	31571	64564	1.38%	0.114%
19	15.827	2158	2166	2176	rBV	2301134	3362017	71.65%	5.914%
20	16.057	2200	2205	2213	rVB4	58271	131190	2.80%	0.231%
21	16.392	2251	2262	2265	rBV4	33841	89448	1.91%	0.157%
22	16.845	2329	2339	2344	rBV5	67688	157300	3.35%	0.277%
23	16.904	2344	2349	2358	rVB2	96443	167731	3.57%	0.295%
24	17.086	2374	2380	2383	rBV	1301902	1825430	38.90%	3.211%
25	17.127	2383	2387	2394	rVV	1539110	2177512	46.41%	3.831%
26	17.215	2394	2402	2409	rVV	361678	576440	12.28%	1.014%
27	17.286	2409	2414	2418	rVB	31803	57777	1.23%	0.102%
28	17.498	2445	2450	2458	rVB	143686	234095	4.99%	0.412%
29	17.962	2525	2529	2531	rBV	122116	165495	3.53%	0.291%
30	17.998	2531	2535	2544	rVV2	589339	1038144	22.12%	1.826%
31	18.092	2548	2551	2556	rVV	79438	114722	2.44%	0.202%
32	18.157	2557	2562	2566	rVV2	304385	497329	10.60%	0.875%
33	18.192	2566	2568	2573	rVB	89205	110902	2.36%	0.195%
34	18.286	2580	2584	2587	rBV2	38314	50100	1.07%	0.088%
35	18.468	2611	2615	2619	rBV	107516	145348	3.10%	0.256%
36	18.515	2619	2623	2629	rVB2	75844	100529	2.14%	0.177%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032724\
Data File : BM044795.D
Acq On : 28 Mar 2024 00:47
Operator : MA/JU
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

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-BM031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.886	2682	2686	2689	rBV	60504	93171	1.99%	0.164%
38	19.033	2707	2711	2717	rVB3	60727	103005	2.20%	0.181%
39	19.151	2725	2731	2740	rBV	2585401	3735646	79.61%	6.571%
40	19.280	2750	2753	2761	rVB2	174839	261696	5.58%	0.460%
41	19.515	2783	2793	2802	rBV	2004825	3550190	75.66%	6.245%
42	19.586	2802	2805	2812	rVB2	92749	146065	3.11%	0.257%
43	19.727	2821	2829	2834	rBV	3414648	4320197	92.07%	7.600%
44	19.839	2844	2848	2850	rBV2	102536	165295	3.52%	0.291%
45	20.015	2875	2878	2882	rVB2	319389	380868	8.12%	0.670%
46	20.115	2891	2895	2899	rBV2	350740	423540	9.03%	0.745%
47	20.209	2909	2911	2915	rVB2	104895	108984	2.32%	0.192%
48	20.927	3031	3033	3037	rVB	147283	165483	3.53%	0.291%
49	21.009	3043	3047	3052	rBV3	555947	813425	17.34%	1.431%
50	21.280	3087	3093	3097	rBV3	1736138	3414569	72.77%	6.007%
51	21.321	3097	3100	3106	rVB	975110	1241833	26.47%	2.185%
52	21.439	3117	3120	3128	rVB2	228016	331567	7.07%	0.583%
53	22.862	3356	3362	3367	rBV2	991969	2339420	49.86%	4.115%
54	23.433	3454	3459	3466	rVB	788308	1466595	31.26%	2.580%
55	23.533	3471	3476	3481	rVV	739555	1308871	27.89%	2.302%

Sum of corrected areas: 56846301

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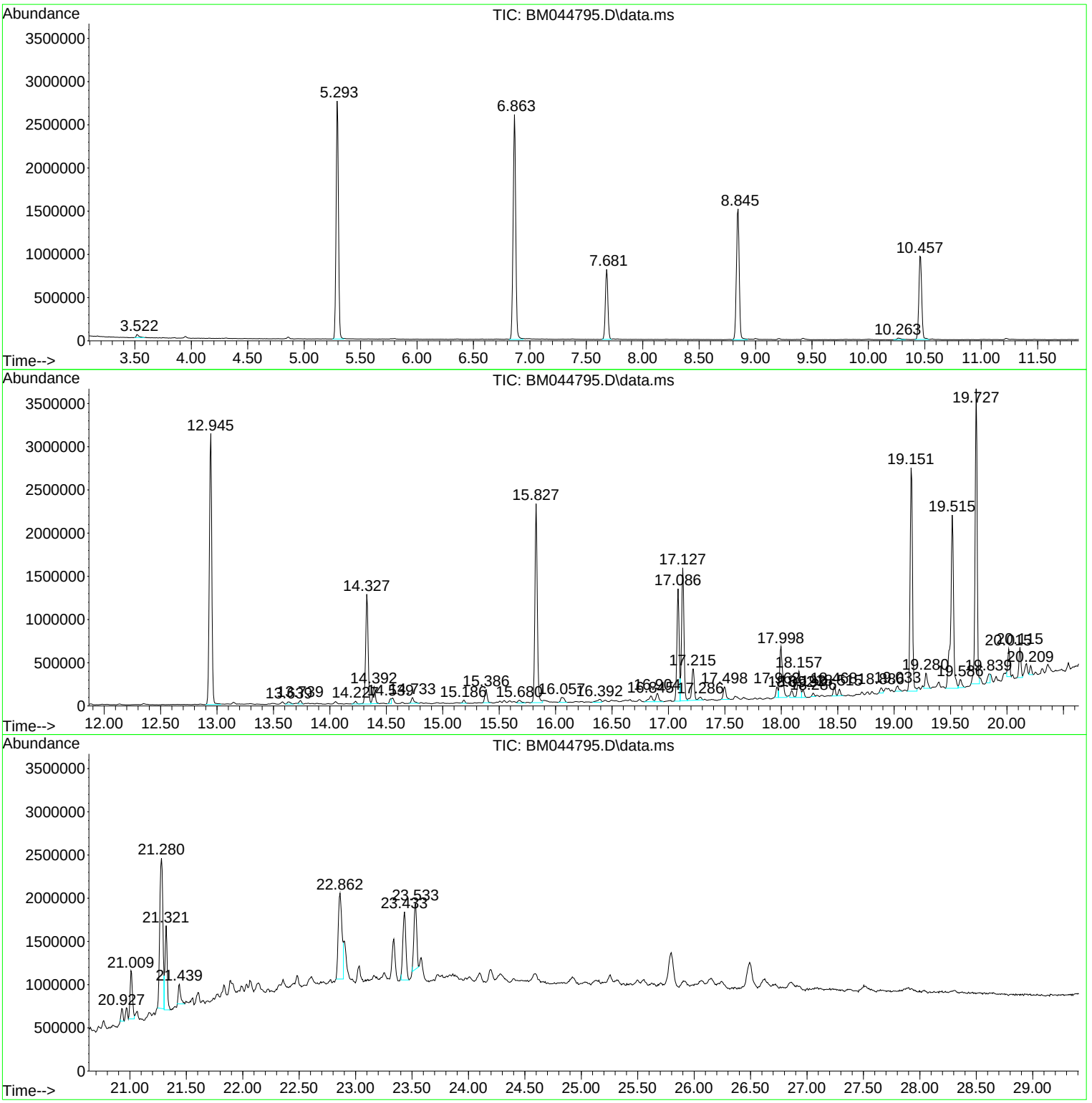
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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\BM032724\
Data File : BM044795.D
Acq On : 28 Mar 2024 00:47
Operator : MA/JU
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

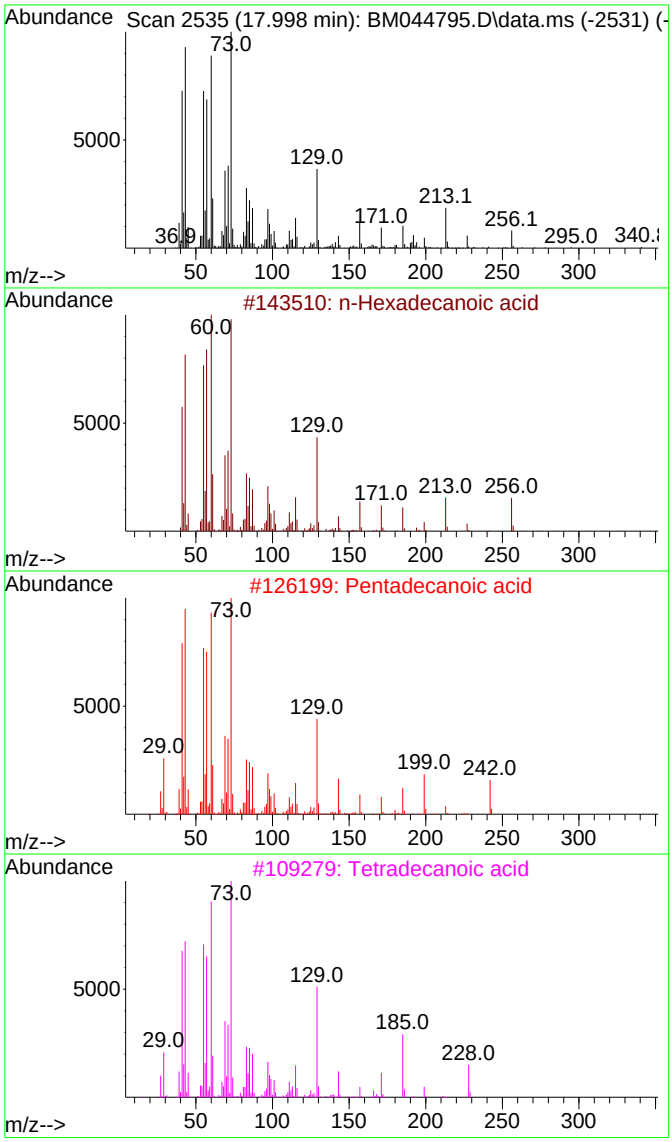
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

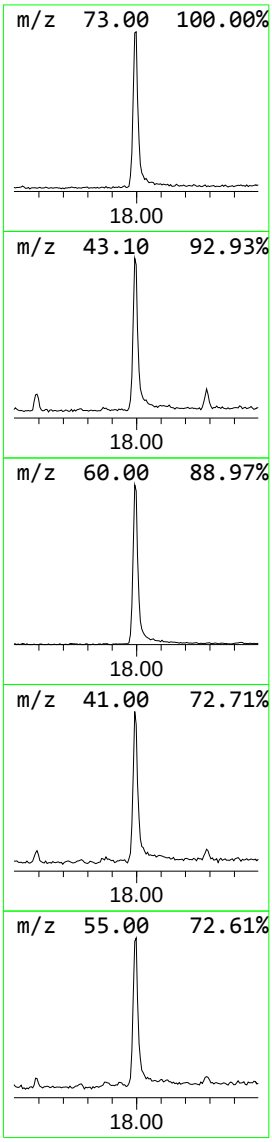
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	11.37 ng	1038140	Phenanthrene-d10	17.086

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





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Data File : BM044795.D
Acq On : 28 Mar 2024 00:47
Operator : MA/JU
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

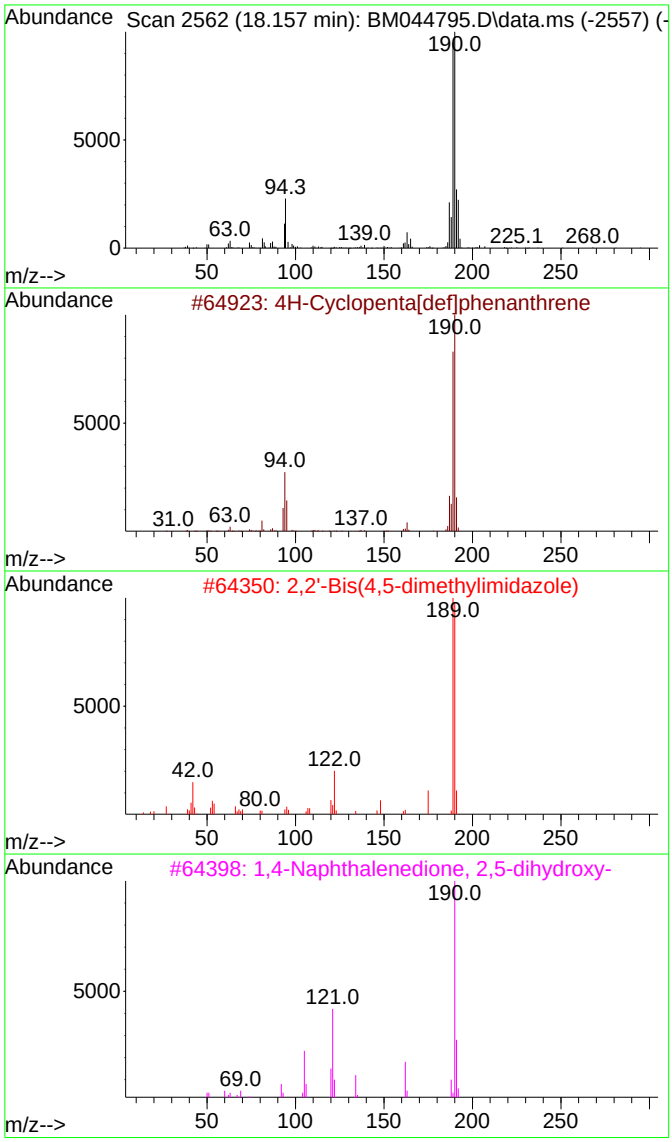
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

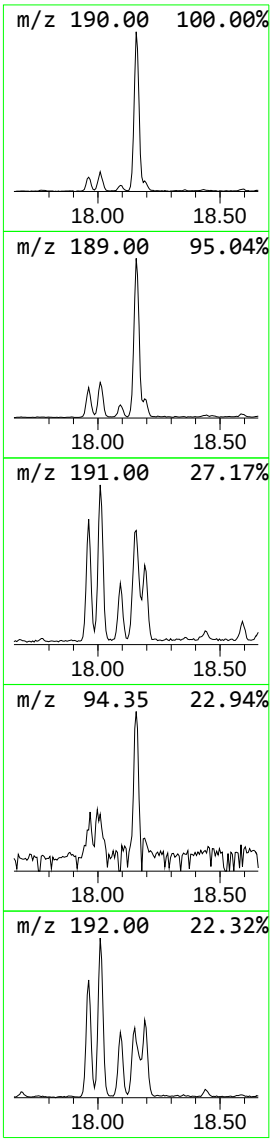
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	5.45 ng	497329	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
3	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032724\
Data File : BM044795.D
Acq On : 28 Mar 2024 00:47
Operator : MA/JU
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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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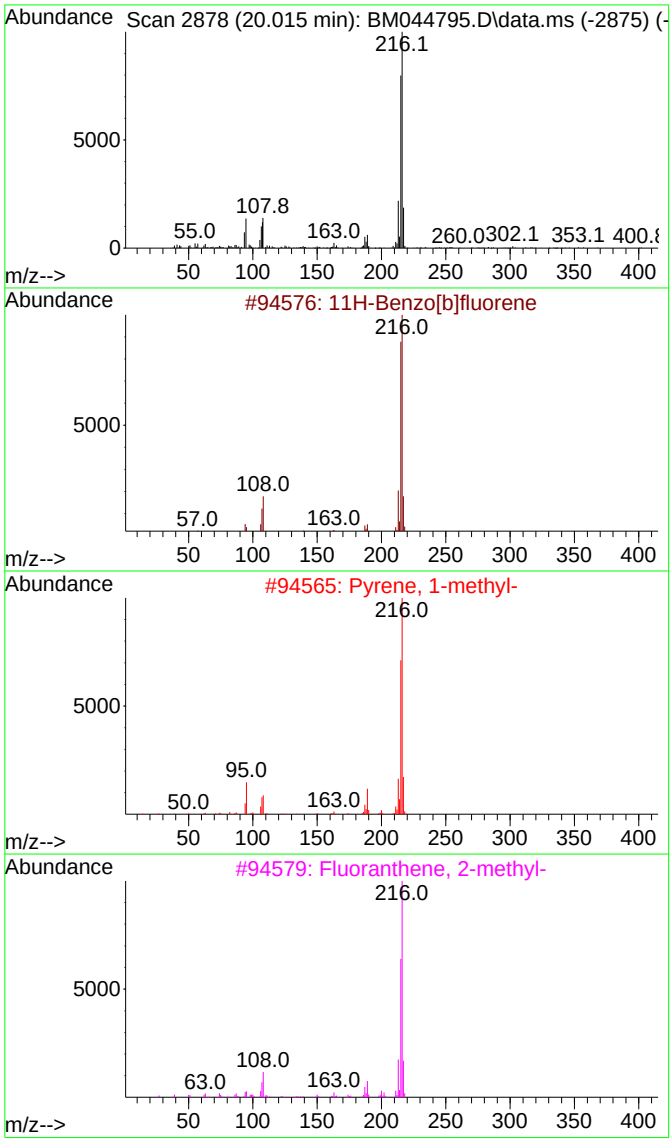
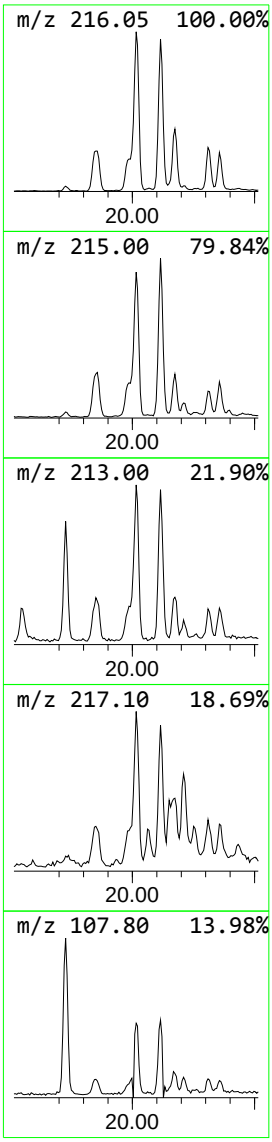
Peak Number 3 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.015	2.23 ng	380868	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032724\
Data File : BM044795.D
Acq On : 28 Mar 2024 00:47
Operator : MA/JU
Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

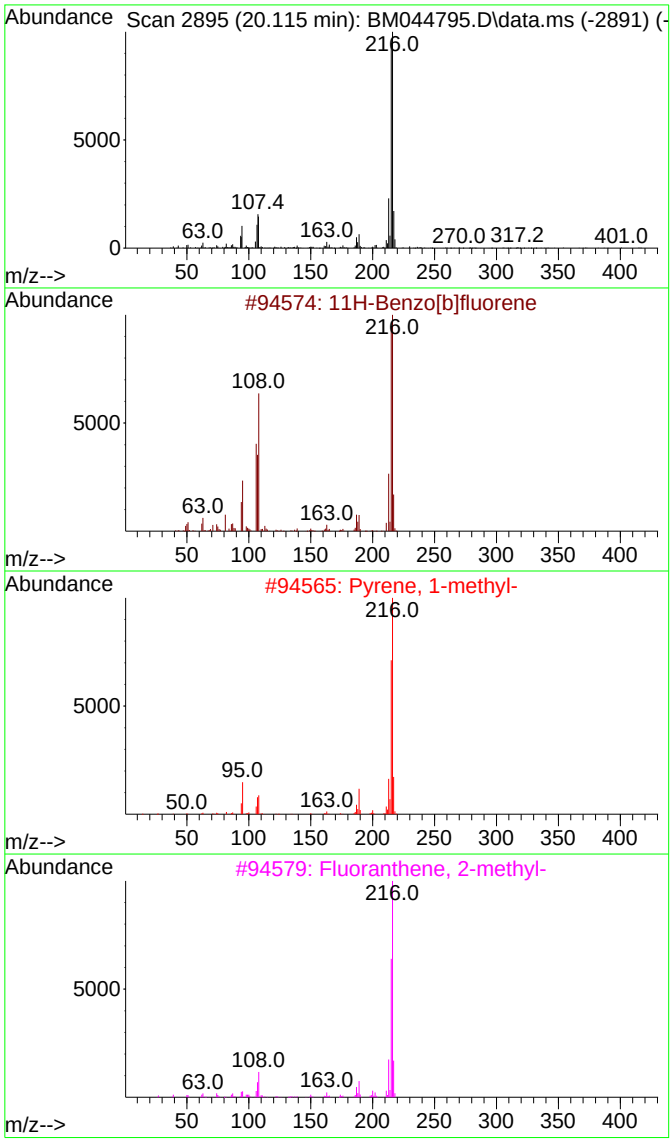
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

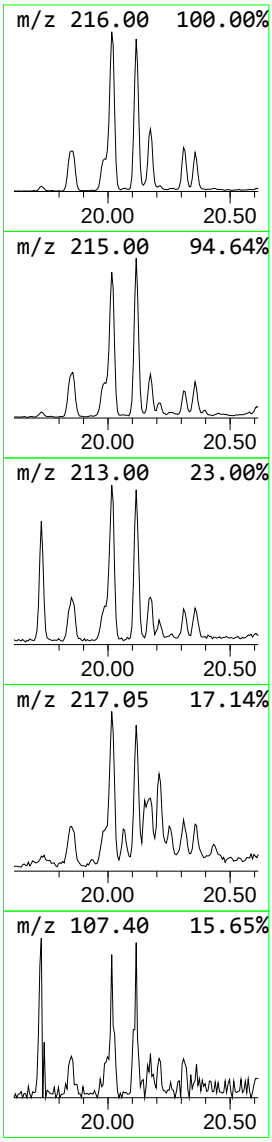
****

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.115	2.48 ng	423540	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





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Data File : BM044795.D
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Sample : P1870-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EXTRA-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

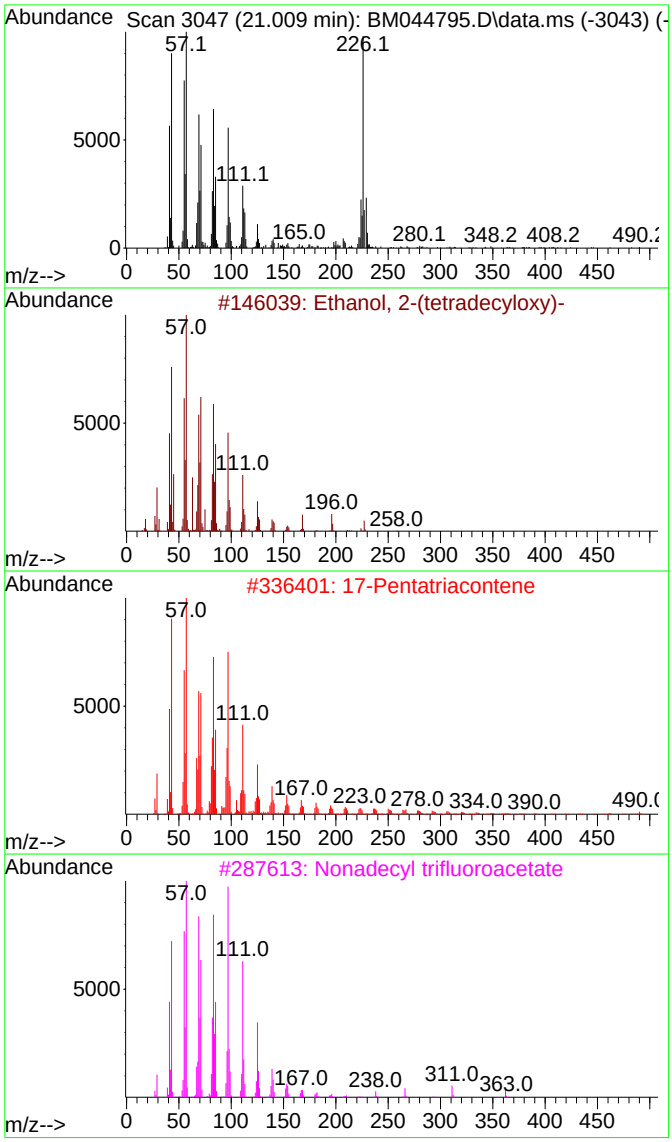
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

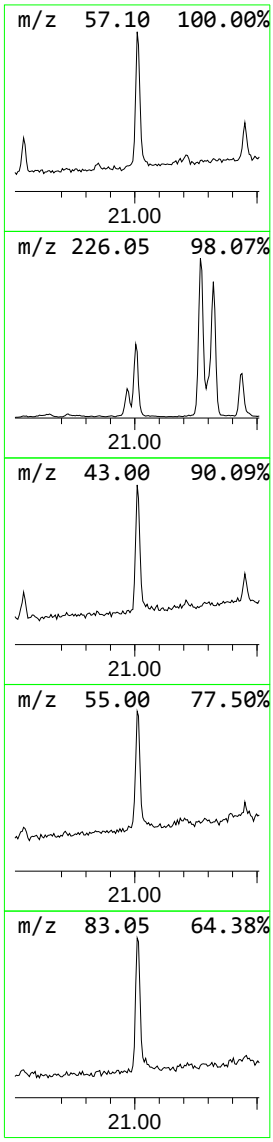
****

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.009	4.76 ng	813425	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	96
2	17-Pentatriacontene	491	C35H70	006971-40-0	78
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	60
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	60
5	Cyclooctacosane	392	C28H56	000297-24-5	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032724\
Data File : BM044795.D
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Operator : MA/JU
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Misc :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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 ...	17.998	11.4	ng	1038140	4	17.086	1825430	20.0
4H-Cyclopenta[d...	18.157	5.5	ng	497329	4	17.086	1825430	20.0
11H-Benzo[b]flu...	20.015	2.2	ng	380868	5	21.286	3414570	20.0
Pyrene, 1-methyl-	20.115	2.5	ng	423540	5	21.286	3414570	20.0
Ethanol, 2-(tet...	21.009	4.8	ng	813425	5	21.286	3414570	20.0