LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032522\
Data File : BM034385.D
Acq On : 25 Mar 2022 15:12
Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200031

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-BM031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034385.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.084	139	144	149	rVB	52920	71772	1.05%	0.144%
2	5.496	377	384	393	rBV	2619601	3733028	54.57%	7.488%
3	7.101	649	657	675	rBV	2286911	3692883	53.98%	7.407%
4	7.831	776	781	789	rVB	56834	93108	1.36%	0.187%
5	7.937	793	799	804	rBV	543068	897843	13.12%	1.801%
6	9.101	990	997	1009	rBV	1438066	2378240	34.76%	4.770%
7	10.754	1269	1278	1283	rBV	645093	1121137	16.39%	2.249%
8	10.801	1283	1286	1296	rVB	75449	128520	1.88%	0.258%
9	12.413	1552	1560	1567	rVB	34026	72114	1.05%	0.145%
10	12.630	1590	1597	1602	rVB	39439	76727	1.12%	0.154%
11	13.207	1688	1695	1707	rBV	3331522	4897370	71.58%	9.823%
12	13.419	1726	1731	1738	rVB2	49807	84109	1.23%	0.169%
13	14.013	1828	1832	1835	rBV2	46122	72681	1.06%	0.146%
14	14.307	1876	1882	1892	rBV	111401	218011	3.19%	0.437%
15	14.419	1897	1901	1908	rVB3	62673	98769	1.44%	0.198%
16	14.583	1920	1929	1935	rBV	878577	1371180	20.04%	2.750%
17	14.648	1935	1940	1948	rVB	171890	284858	4.16%	0.571%
18	14.983	1992	1997	2002	rBV	78722	122654	1.79%	0.246%
19	15.183	2015	2031	2033	rBV3	119875	429318	6.28%	0.861%
20	15.630	2102	2107	2118	rVB	117556	225653	3.30%	0.453%
21	16.066	2175	2181	2189	rBV	2410118	3566163	52.13%	7.153%
22	16.313	2216	2223	2228	rBV4	47256	121923	1.78%	0.245%
23	17.142	2360	2364	2373	rVB2	72570	118807	1.74%	0.238%
24	17.324	2389	2395	2398	rBV	1033572	1456717	21.29%	2.922%
25	17.365	2398	2402	2407	rVB	848913	1155549	16.89%	2.318%
26	17.454	2413	2417	2423	rVB	257554	371562	5.43%	0.745%
27	18.218	2541	2547	2550	rBV2	198978	367269	5.37%	0.737%
28	18.401	2573	2578	2582	rBV2	230170	377379	5.52%	0.757%
29	19.383	2740	2745	2750	rVB	1762270	2261265	33.05%	4.536%
30	19.742	2797	2806	2814	rBV	1605912	2686078	39.26%	5.388%
31	19.942	2835	2840	2845	rBV	5666139	6841384	100.00%	13.722%
32	20.236	2886	2890	2896	rVB	289834	427066	6.24%	0.857%
33	20.330	2903	2906	2913	rBV2	229077	400338	5.85%	0.803%
34	21.200	3050	3054	3063	rVB4	502005	896020	13.10%	1.797%
35	21.406	3086	3089	3093	rVB	569844	593342	8.67%	1.190%
36	21.495	3098	3104	3108	rVV2	1638814	3058423	44.70%	6.135%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032522\
Data File : BM034385.D
Acq On : 25 Mar 2022 15:12
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RBR-200031

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-BM031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.536	3108	3111	3121	rVB	653204	1003171	14.66%	2.012%
38	23.177	3386	3390	3396	rBV2	813217	1588292	23.22%	3.186%
39	23.812	3493	3498	3505	rVB	503107	988000	14.44%	1.982%
40	23.918	3511	3516	3522	rBV2	811472	1506862	22.03%	3.022%

Sum of corrected areas: 49855585

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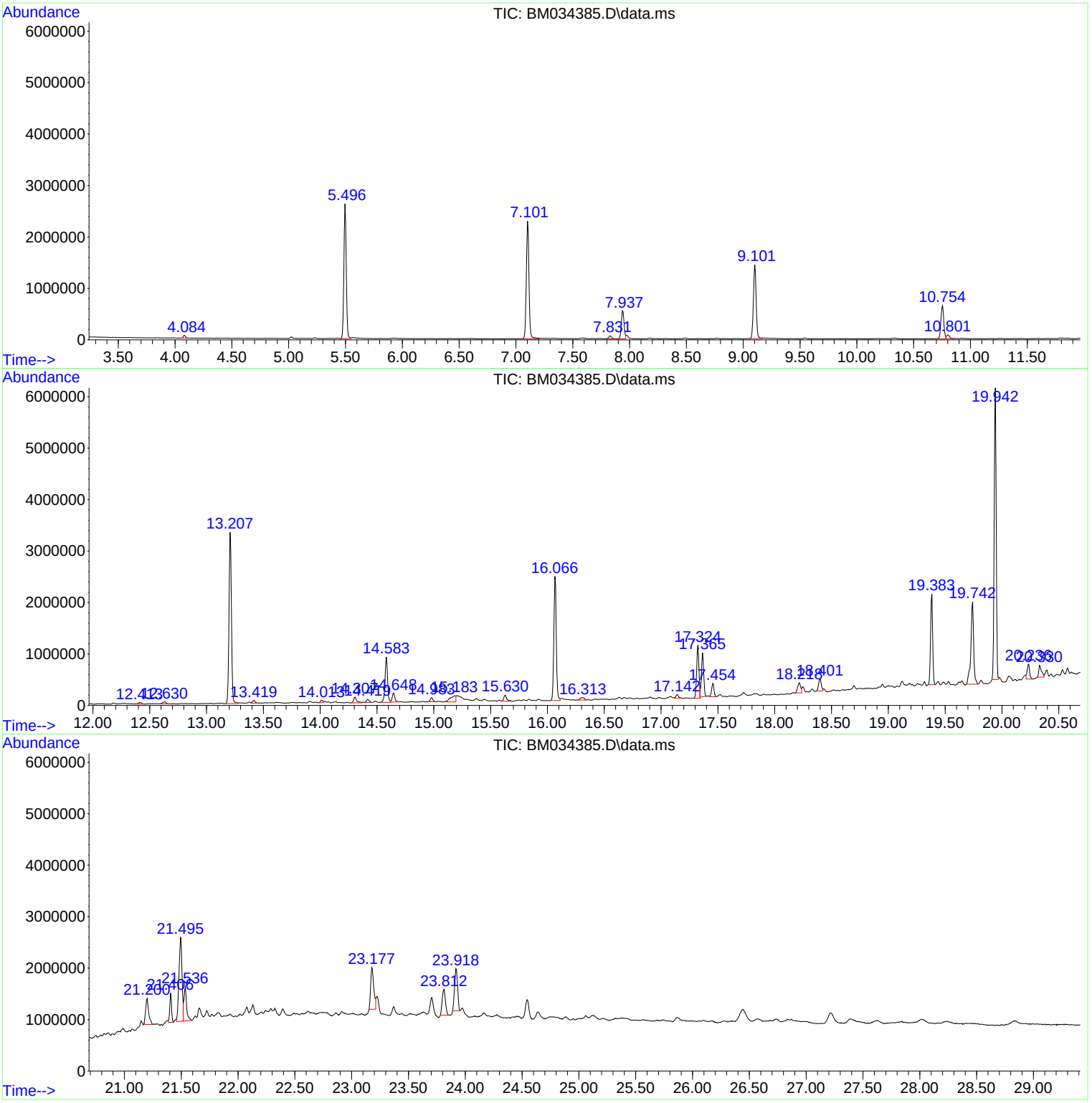
Acq On : 25 Mar 2022 15:12
Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200031

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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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Data File : BM034385.D
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Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200031

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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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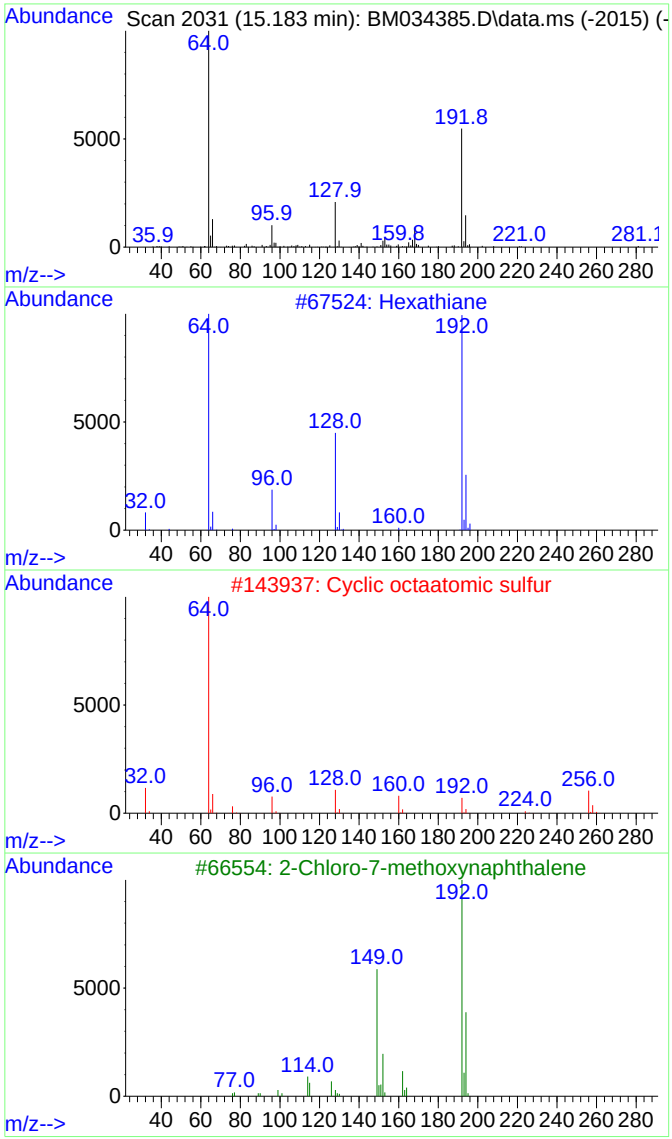
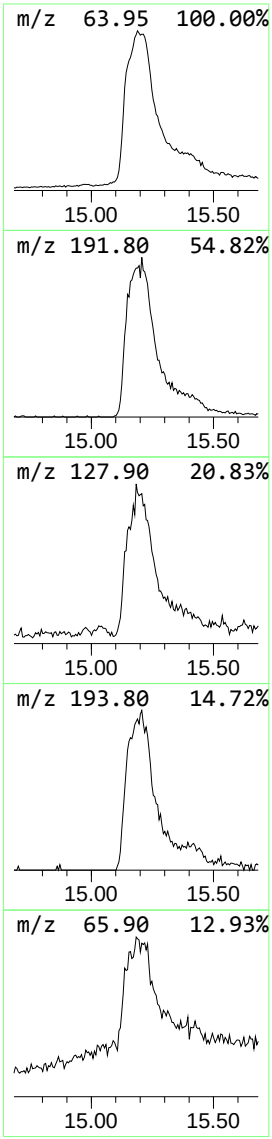
Peak Number 2 Hexathiane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.183	6.26 ng	429318	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	Cyclic octaatomic sulfur	256	S8	010544-50-0	9
3	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	7
4	Methanesulfonamide, 1-chloro-	129	CH4ClNO2S	021335-43-3	5
5	dimethyl tellurenyl	192	C2H6STe	1000374-19-6	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032522\
Data File : BM034385.D
Acq On : 25 Mar 2022 15:12
Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200031

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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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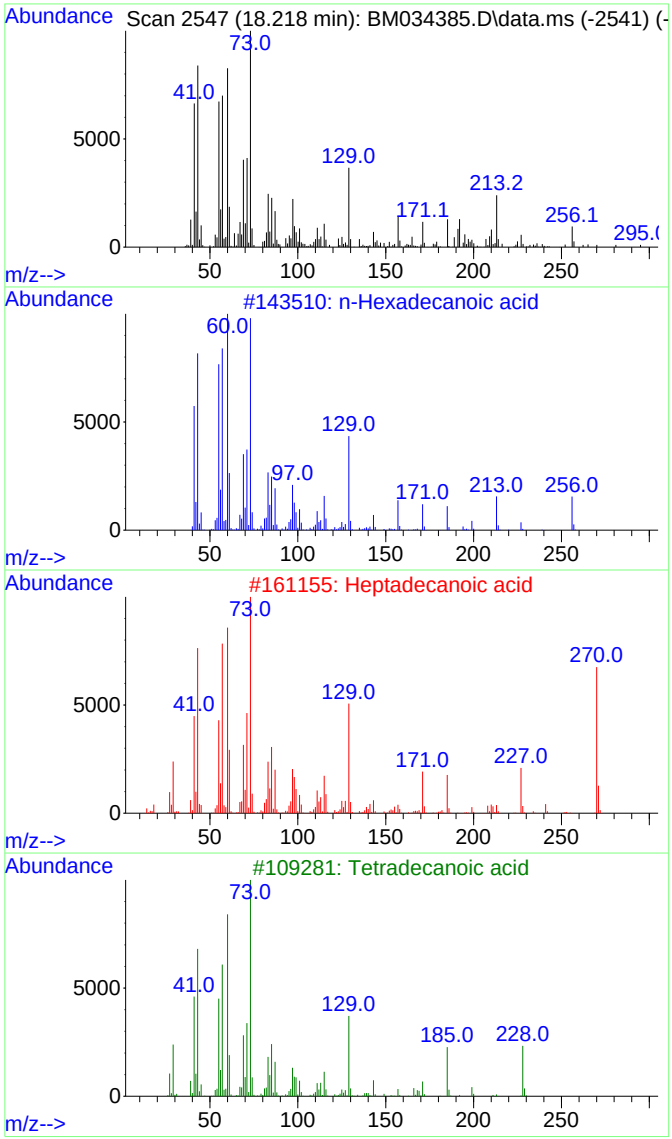
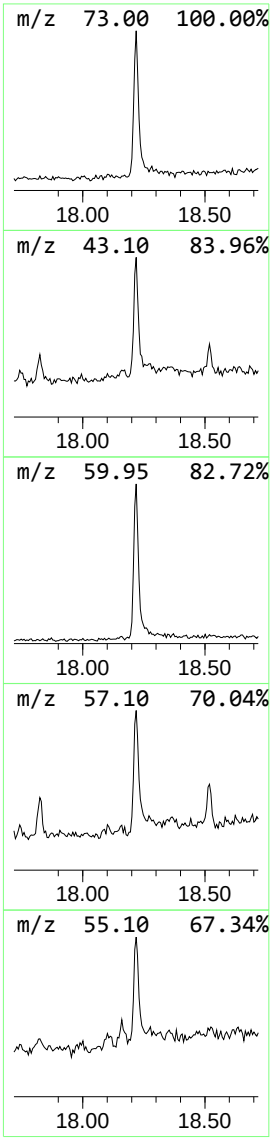
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	5.04 ng	367269	Phenanthrene-d10	17.324

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032522\
Data File : BM034385.D
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Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200031

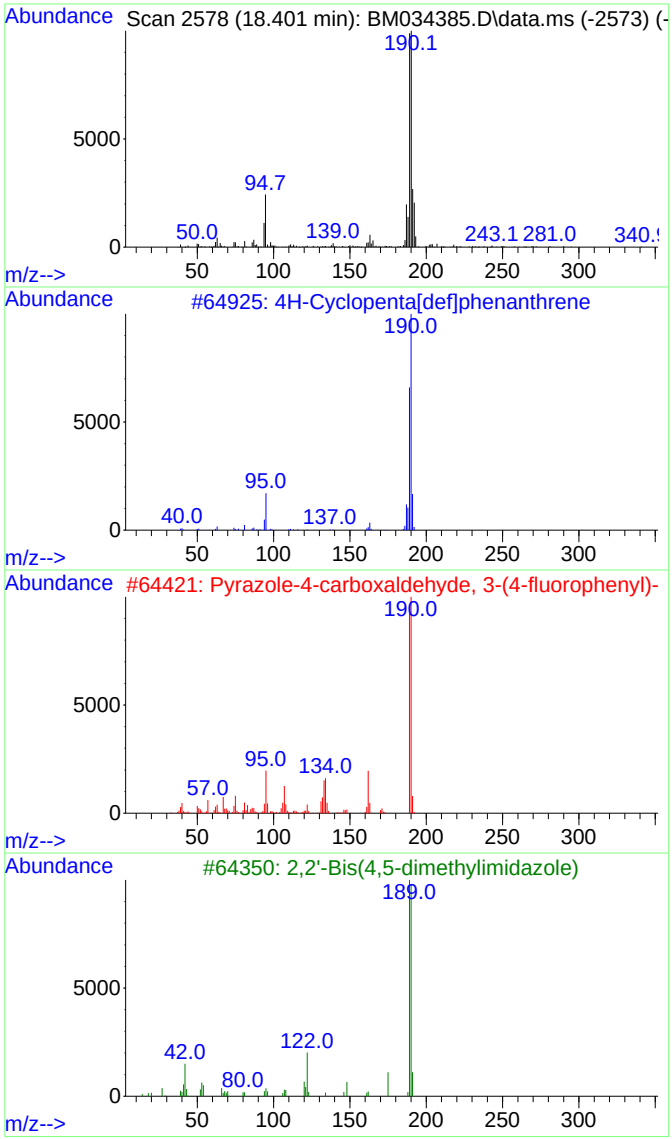
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

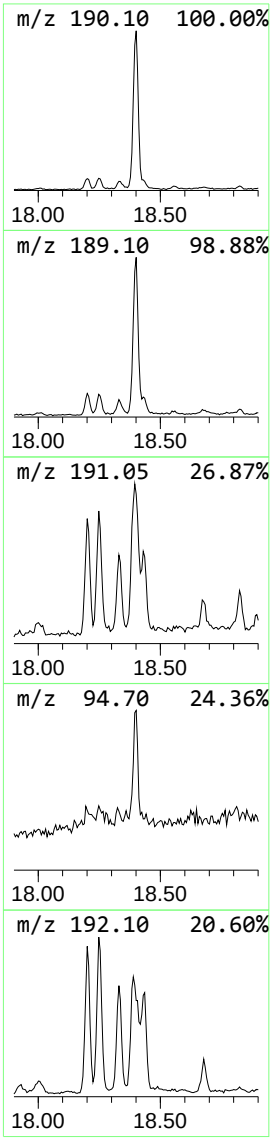
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.401	5.18 ng	377379	Phenanthrene-d10	17.324

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	42
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	Methyl diselenide	190	C2H6Se2	007101-31-7	35
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032522\
Data File : BM034385.D
Acq On : 25 Mar 2022 15:12
Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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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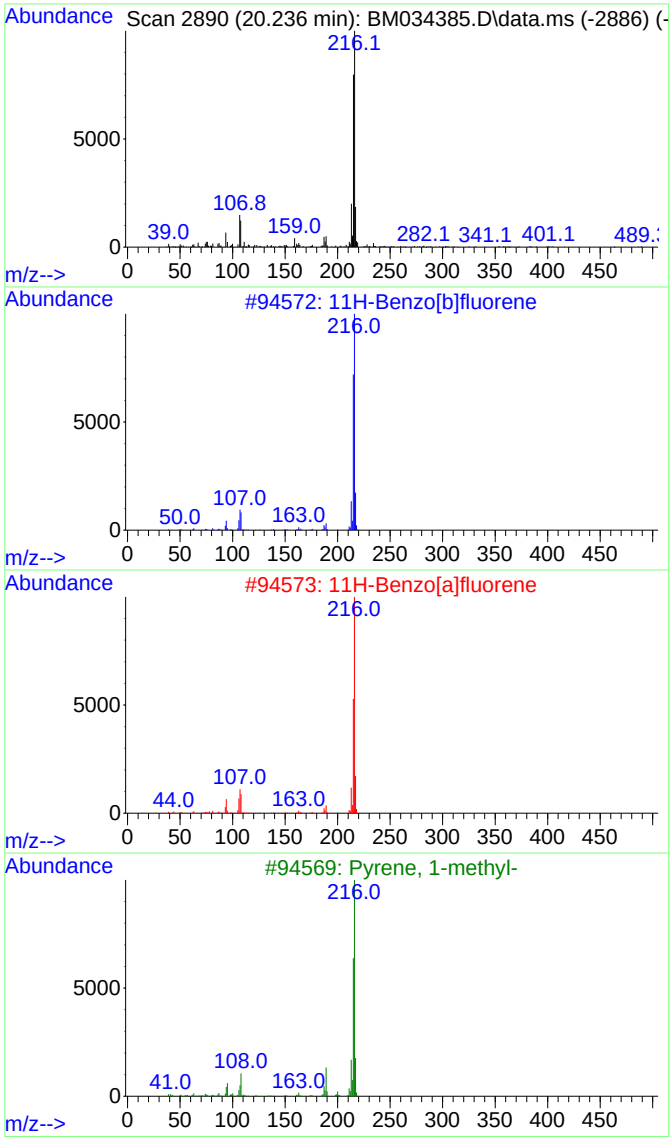
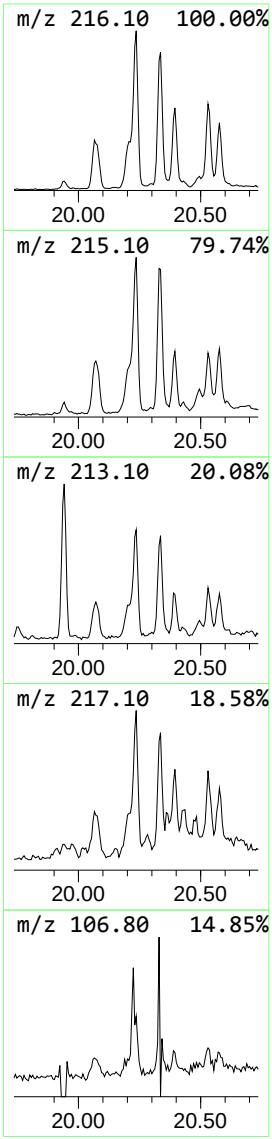
Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.236	2.79 ng	427066	Chrysene-d12	21.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	97
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	72
4	Pyrene, 4-methyl-	216	C17H12	003353-12-6	60
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032522\
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Acq On : 25 Mar 2022 15:12
Operator : CG/JU
Sample : N2103-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200031

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

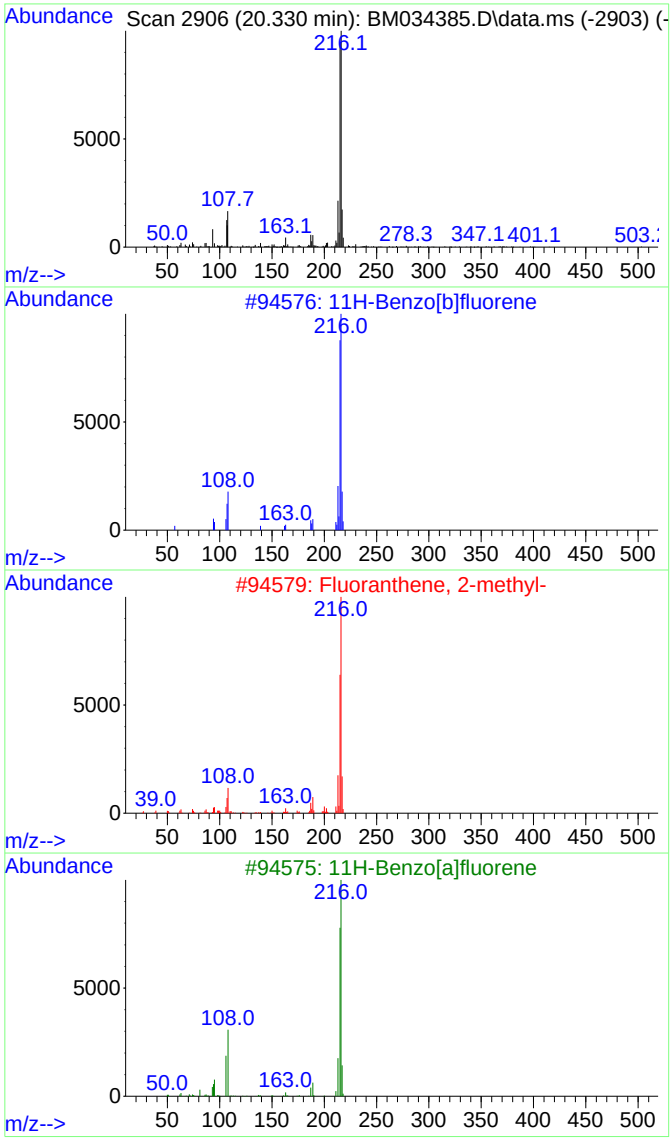
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

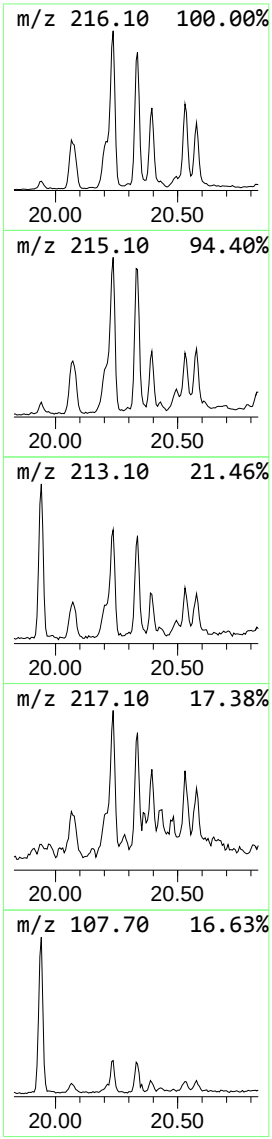
****

Peak Number 6 Fluoranthene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.330	2.62 ng	400338	Chrysene-d12	21.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	74
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	72
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	68





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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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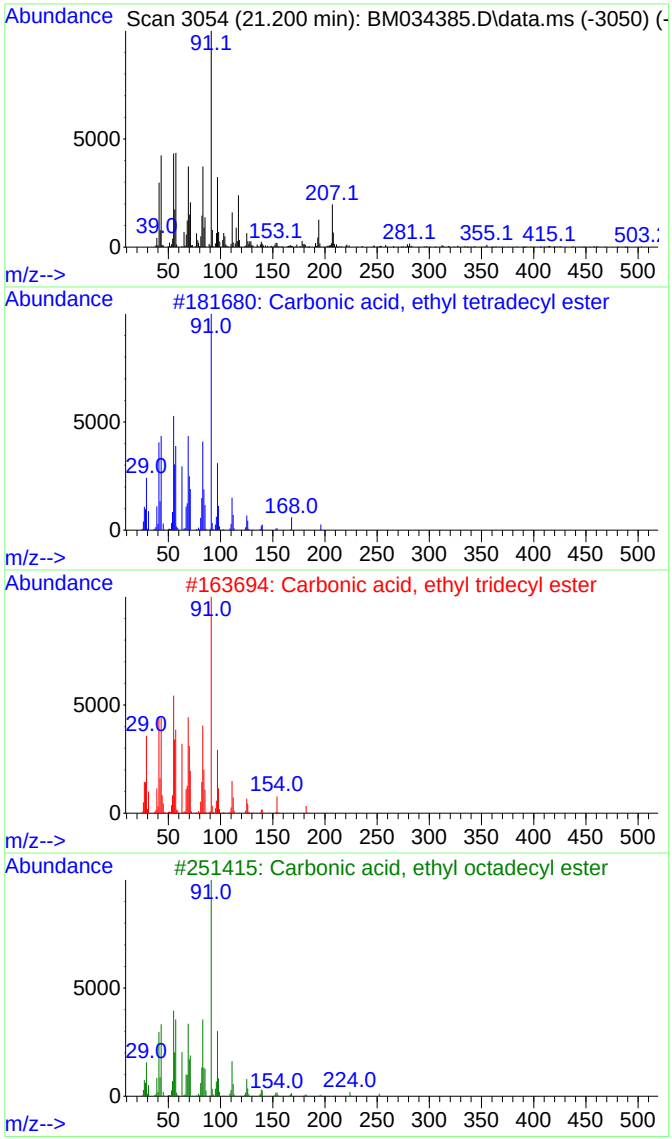
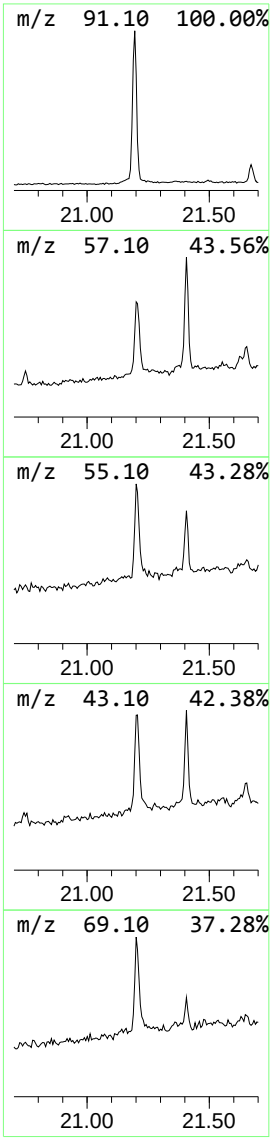
Peak Number 7 unknown21.201 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.201	5.86 ng	896020	Chrysene-d12	21.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, ethyl tetradecyl ...	286	C17H34O3	1000314-59-4	35
2	Carbonic acid, ethyl tridecyl ester	272	C16H32O3	1000314-59-3	35
3	Carbonic acid, ethyl octadecyl e...	342	C21H42O3	1000314-59-8	35
4	Docosyl ethyl carbonate	398	C25H50O3	1000373-79-2	35
5	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	30





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.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
Hexathiane	15.183	6.3	ng	429318	3	14.583	1371180	20.0
n-Hexadecanoic ...	18.218	5.0	ng	367269	4	17.324	1456720	20.0
4H-Cyclopenta[d...	18.401	5.2	ng	377379	4	17.324	1456720	20.0
11H-Benzo[b]flu...	20.236	2.8	ng	427066	5	21.500	3058420	20.0
Fluoranthene, 2...	20.330	2.6	ng	400338	5	21.500	3058420	20.0
unknown21.201	21.201	5.9	ng	896020	5	21.500	3058420	20.0