LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047970.D
Acq On : 22 Jan 2021 2:08
Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BORE-2-ALT

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_G\METHODS\8270-BG012121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047970.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.700	396	402	414	rVB	774896	1203749	54.80%	6.884%
2	7.293	665	673	683	rVB	747650	1297232	59.05%	7.418%
3	7.727	739	747	754	rBV	16883	26948	1.23%	0.154%
4	8.145	811	818	825	rBV	184196	307749	14.01%	1.760%
5	9.308	1006	1016	1026	rVB	478237	821203	37.38%	4.696%
6	10.959	1288	1297	1304	rBV	238880	439429	20.00%	2.513%
7	12.610	1572	1578	1586	rVB	33891	51626	2.35%	0.295%
8	12.821	1608	1614	1621	rBV	15771	27767	1.26%	0.159%
9	13.397	1703	1712	1720	rBV	1008431	1553687	70.73%	8.885%
10	14.214	1844	1851	1856	rBV	70883	105429	4.80%	0.603%
11	14.766	1937	1945	1951	rBV	404330	645777	29.40%	3.693%
12	14.831	1951	1956	1963	rVB	39063	61400	2.80%	0.351%
13	15.166	2007	2013	2017	rBV	30495	43016	1.96%	0.246%
14	15.812	2116	2123	2130	rBV2	39169	57844	2.63%	0.331%
15	16.247	2191	2197	2204	rBV	1044201	1560419	71.03%	8.923%
16	17.510	2406	2412	2416	rBV	539810	805518	36.67%	4.606%
17	17.551	2416	2419	2425	rVV	129910	191089	8.70%	1.093%
18	17.645	2429	2435	2440	rVB2	30648	55022	2.50%	0.315%
19	17.904	2470	2479	2484	rBV3	15479	33974	1.55%	0.194%
20	18.391	2556	2562	2567	rBV3	169885	253147	11.52%	1.448%
21	18.433	2567	2569	2577	rVB2	28960	41952	1.91%	0.240%
22	18.579	2588	2594	2599	rBV2	40251	75026	3.42%	0.429%
23	19.555	2754	2760	2766	rVB	382257	520869	23.71%	2.979%
24	19.655	2773	2777	2783	rBV3	83299	118686	5.40%	0.679%
25	19.796	2799	2801	2806	rVB5	18785	25483	1.16%	0.146%
26	19.884	2811	2816	2817	rBV2	70986	85852	3.91%	0.491%
27	19.913	2817	2821	2829	rVV	285324	426466	19.41%	2.439%
28	20.113	2848	2855	2860	rBV	1644138	2196751	100.00%	12.562%
29	20.230	2870	2875	2877	rBV3	22542	38143	1.74%	0.218%
30	20.407	2898	2905	2910	rVB	62984	117034	5.33%	0.669%
31	20.507	2917	2922	2926	rBV	59801	79336	3.61%	0.454%
32	20.559	2926	2931	2934	rVV4	27918	43524	1.98%	0.249%
33	20.601	2934	2938	2941	rVB3	25909	36030	1.64%	0.206%
34	21.106	3019	3024	3029	rVB	233783	271052	12.34%	1.550%
35	21.370	3064	3069	3071	rBV2	23839	35636	1.62%	0.204%
36	21.429	3072	3079	3089	rVV5	232611	420197	19.13%	2.403%

LSC Area Percent Report

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Data File : BG047970.D
Acq On : 22 Jan 2021 2:08
Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BORE-2-ALT

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_G\METHODS\8270-BG012121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.523	3093	3095	3101	rVB3	47944	67824	3.09%	0.388%
38	21.793	3132	3141	3146	rBV3	570300	1248957	56.85%	7.142%
39	21.840	3146	3149	3155	rVB	143889	214740	9.78%	1.228%
40	21.999	3172	3176	3182	rVB3	39500	70464	3.21%	0.403%
41	22.205	3207	3211	3215	rBV3	24349	42952	1.96%	0.246%
42	22.252	3215	3219	3226	rVB4	73246	122808	5.59%	0.702%
43	22.769	3304	3307	3311	rVB4	35421	47271	2.15%	0.270%
44	24.044	3517	3524	3533	rBV3	91762	309803	14.10%	1.772%
45	24.790	3644	3651	3659	rVB2	48375	125443	5.71%	0.717%
46	24.943	3670	3677	3685	rVB	75186	194643	8.86%	1.113%
47	25.101	3695	3704	3712	rBV2	302487	856428	38.99%	4.897%
48	26.482	3932	3939	3952	rVB2	30787	111855	5.09%	0.640%

Sum of corrected areas: 17487250

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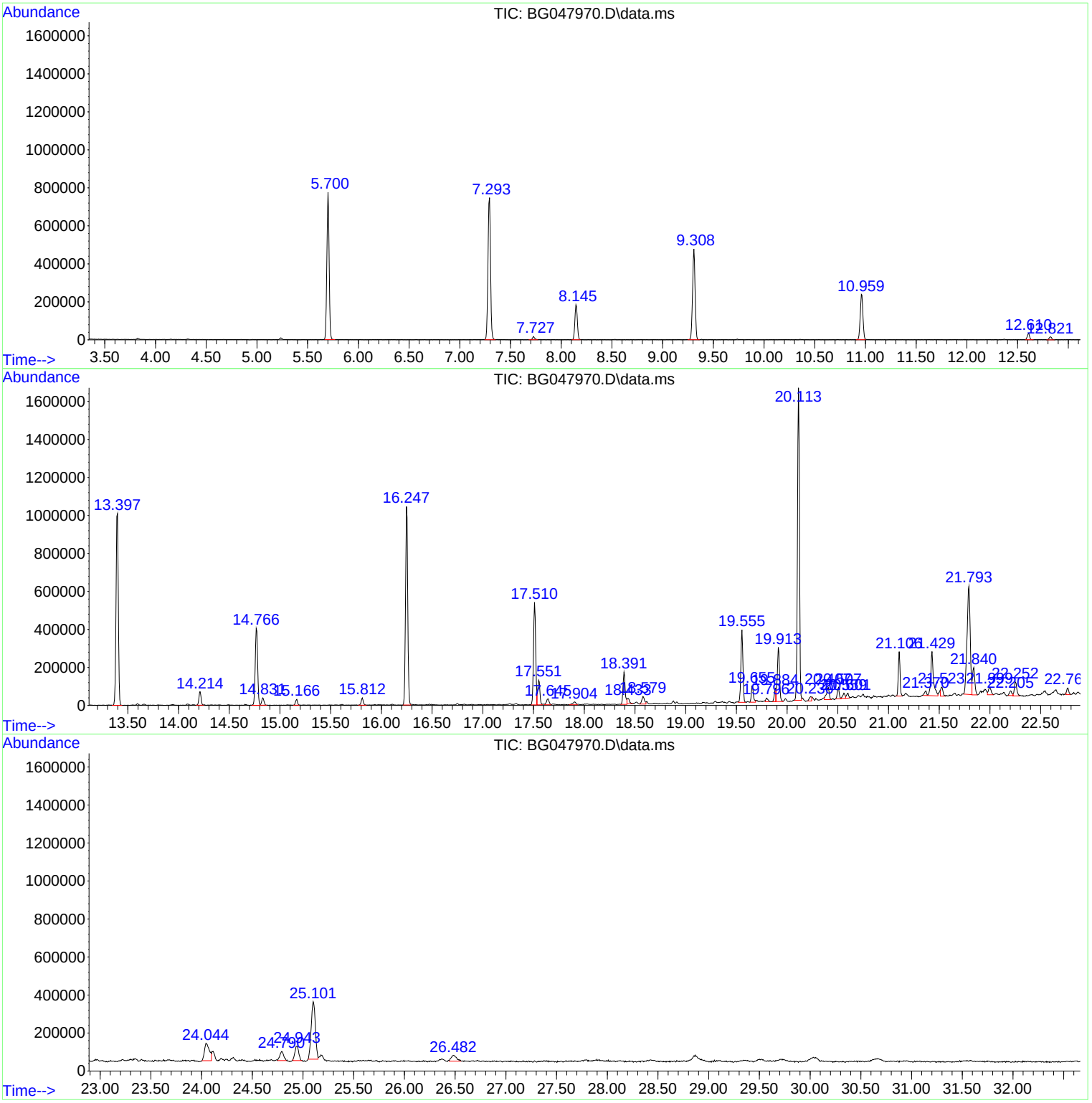
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BORE-2-ALT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047970.D
Acq On : 22 Jan 2021 2:08
Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BORE-2-ALT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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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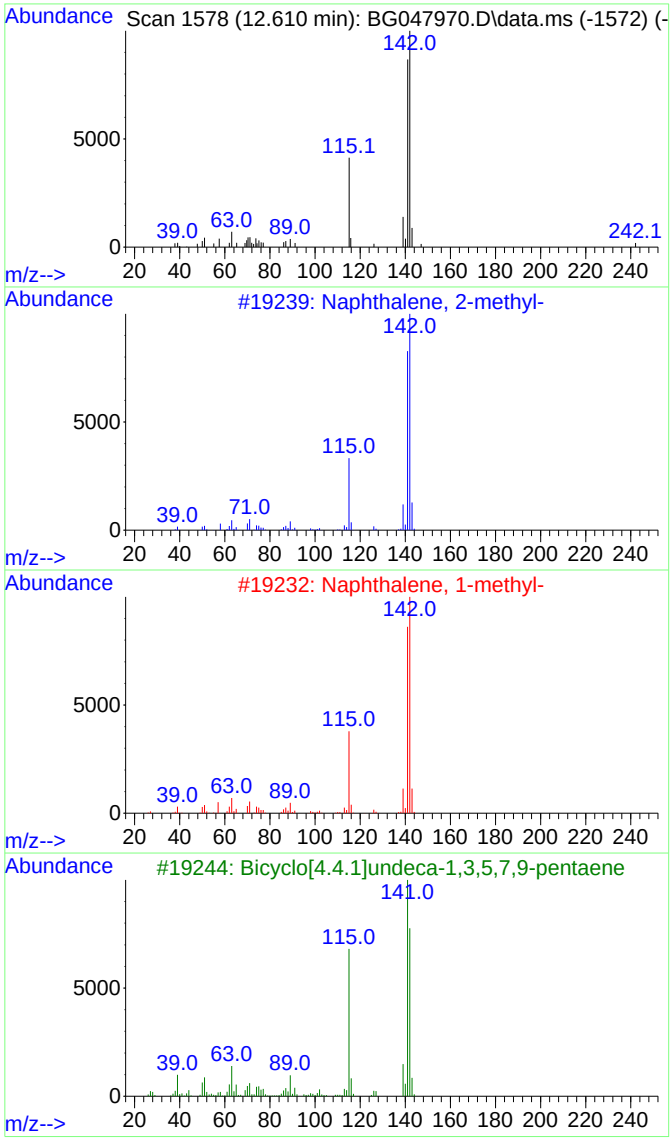
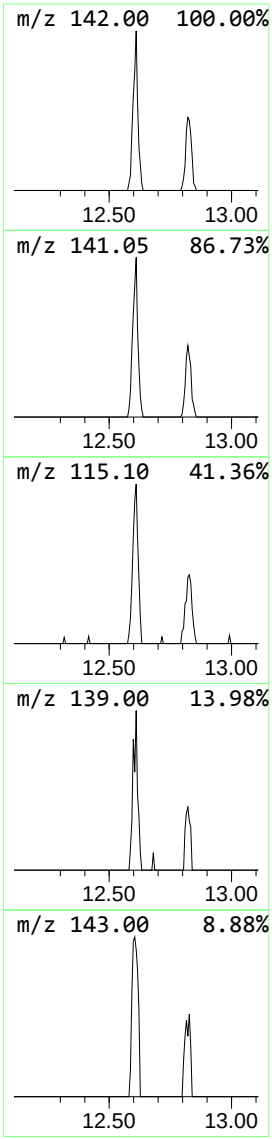
Peak Number 1 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	2.35 ng	51626	Naphthalene-d8	10.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
3	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047970.D
Acq On : 22 Jan 2021 2:08
Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BORE-2-ALT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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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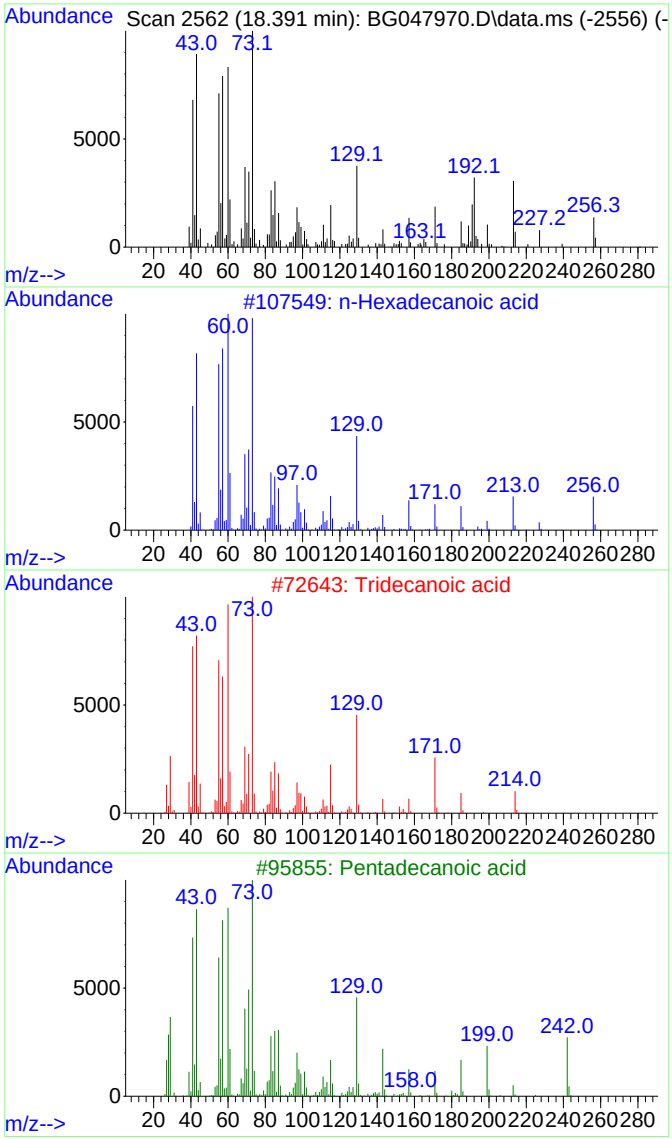
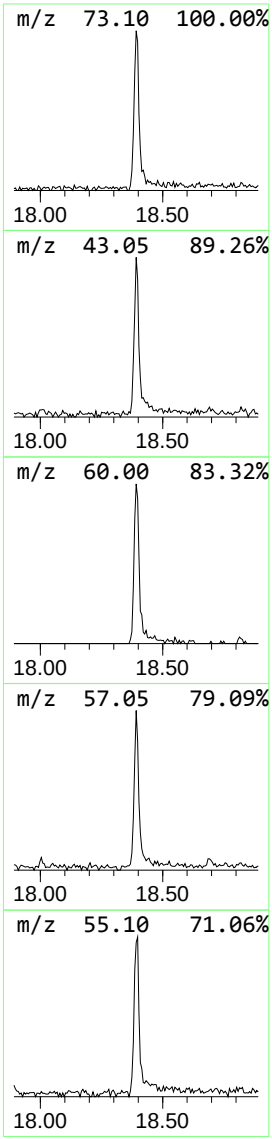
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.391	6.29 ng	253147	Phenanthrene-d10	17.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047970.D
Acq On : 22 Jan 2021 2:08
Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BORE-2-ALT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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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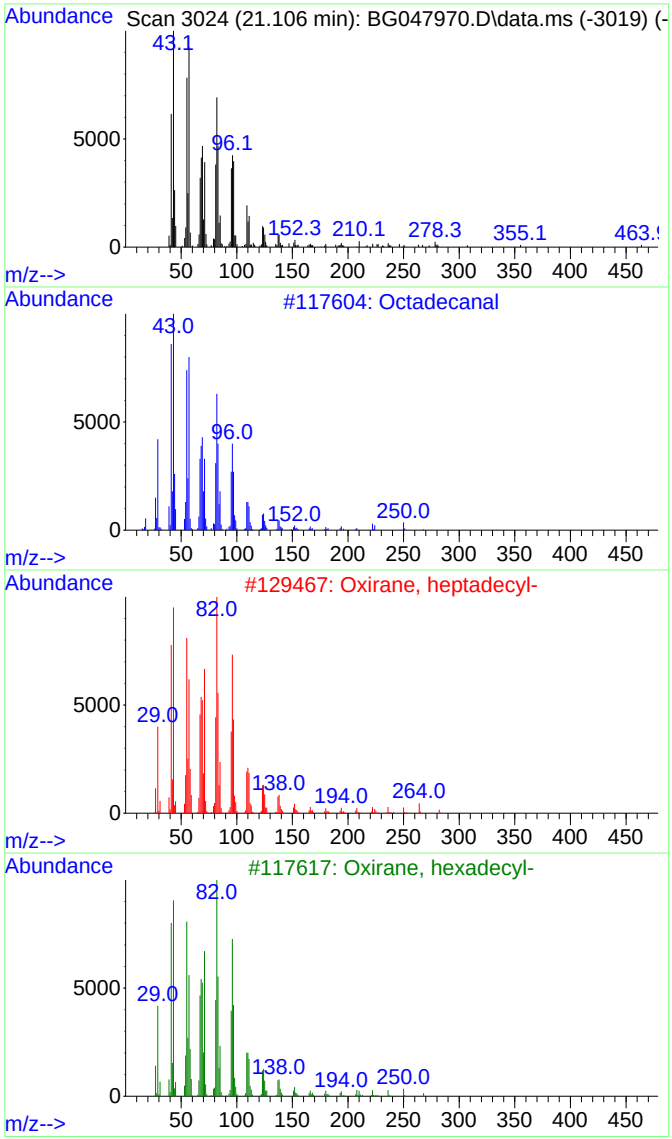
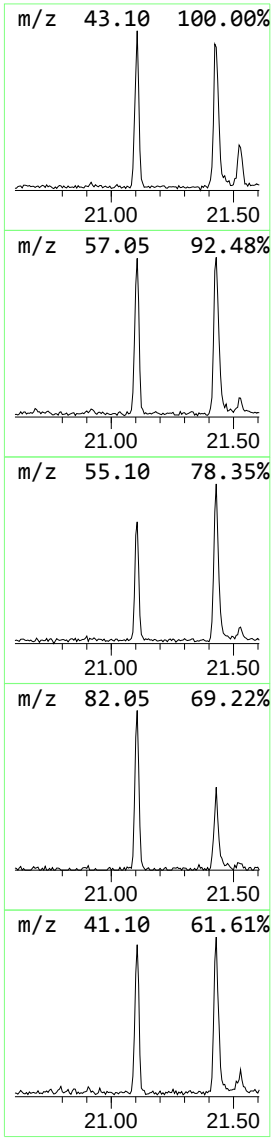
Peak Number 3 Octadecanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.106	4.34 ng	271052	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	87
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
4	1,19-Eicosadiene	278	C20H38	014811-95-1	68
5	Tetradecanal	212	C14H28O	000124-25-4	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047970.D
Acq On : 22 Jan 2021 2:08
Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BORE-2-ALT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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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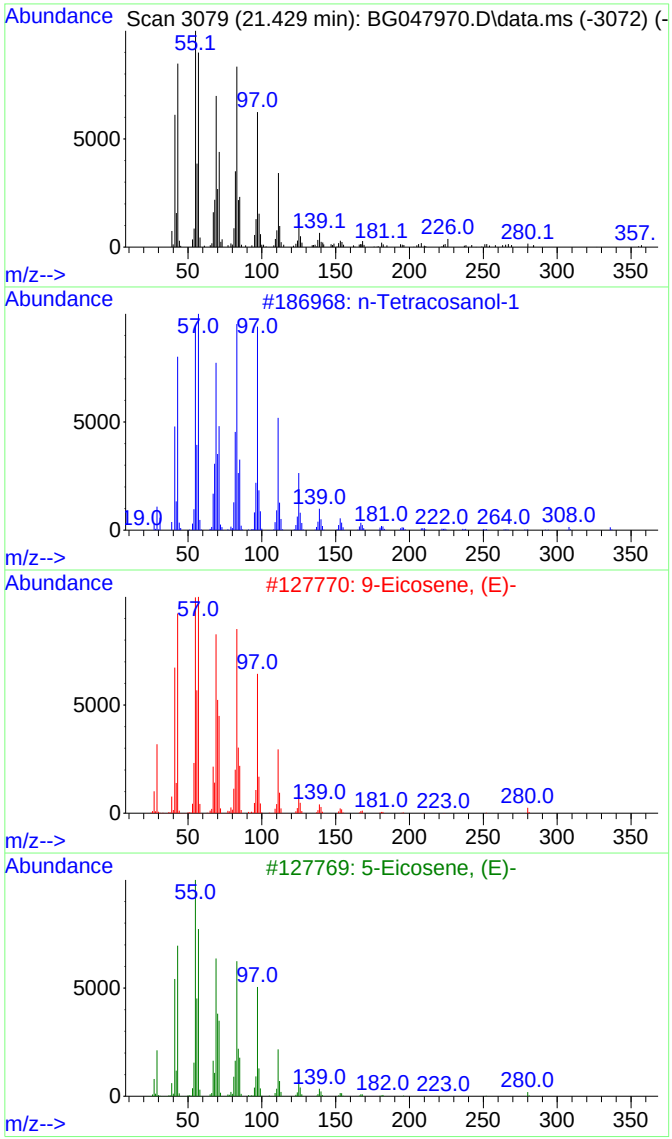
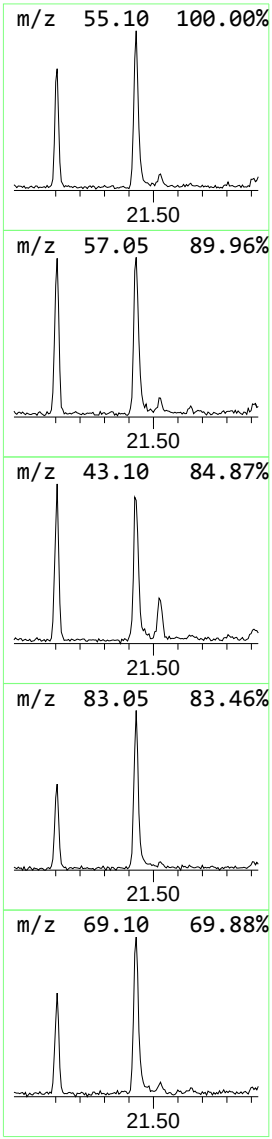
Peak Number 4 n-Tetracosanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.429	6.73 ng	420197	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	1-Tricosene	322	C23H46	018835-32-0	91





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Operator : CG/JU
Sample : M1159-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BORE-2-ALT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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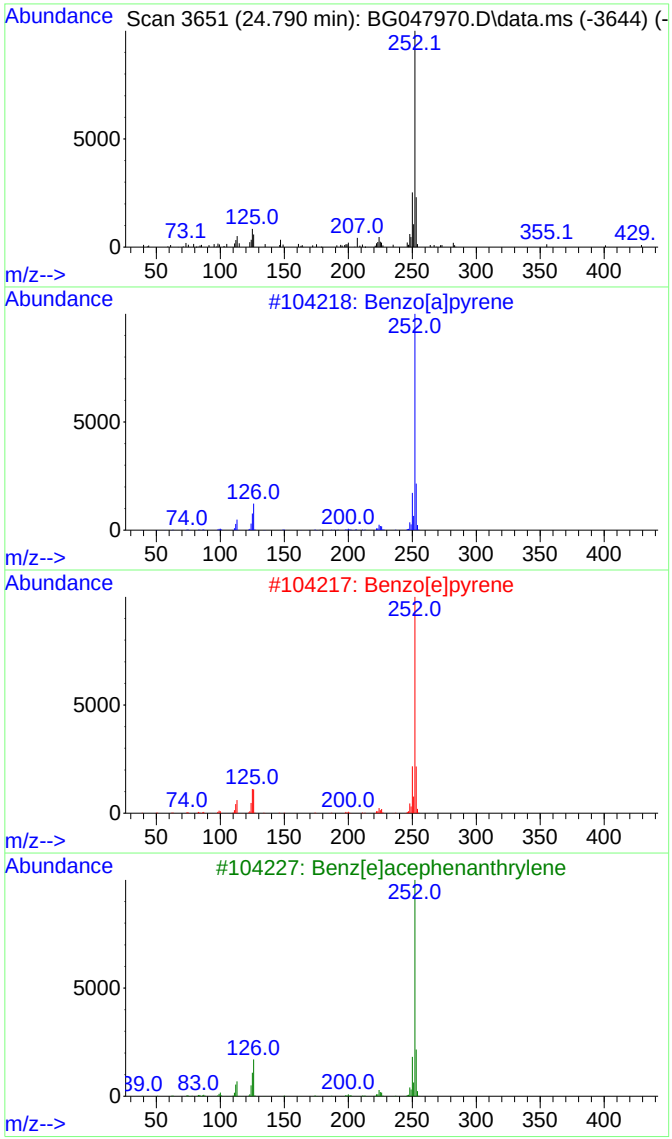
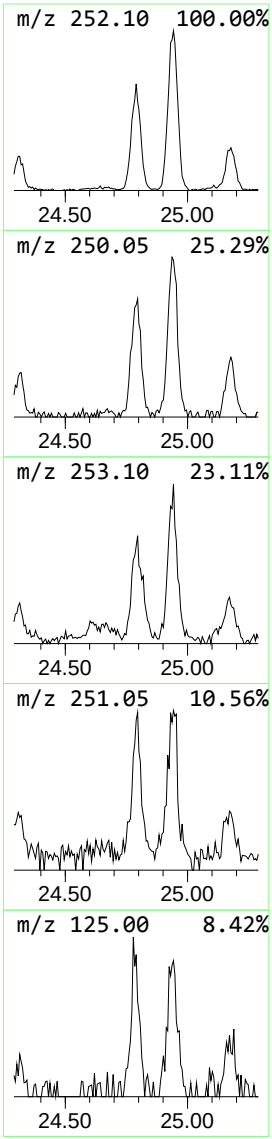
Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.790	2.93 ng	125443	Perylene-d12	25.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	90
2	Benzo[e]pyrene	252	C20H12	000192-97-2	81
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
4	Perylene	252	C20H12	000198-55-0	76
5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72





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BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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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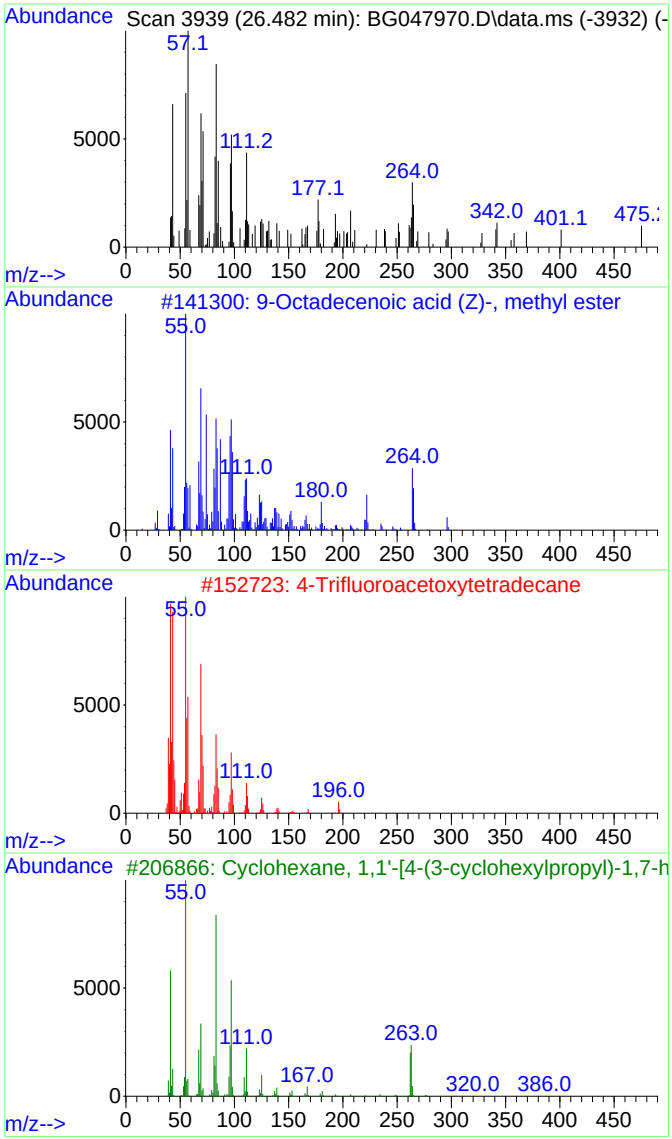
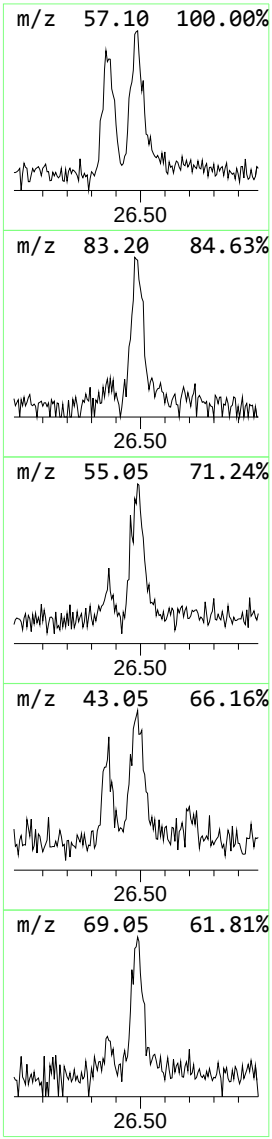
Peak Number 6 unknown26.482 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.482	2.61 ng	111855	Perylene-d12	25.101

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	38
2	4-Trifluoroacetoxytetradecane	310	C16H29F3O2	1000245-47-6	38
3	Cyclohexane, 1,1'-[4-(3-cyclohex...	388	C28H52	055334-73-1	37
4	Tetradecanoic acid, 2-hydroxy-, ...	258	C15H30O3	056009-40-6	32
5	Oleic Acid	282	C18H34O2	000112-80-1	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
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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
Naphthalene, 1-...	12.610	2.4	ng	51626	2	10.965	439429	20.0
n-Hexadecanoic ...	18.391	6.3	ng	253147	4	17.510	805518	20.0
Octadecanal	21.106	4.3	ng	271052	5	21.793	1248960	20.0
n-Tetracosanol-1	21.429	6.7	ng	420197	5	21.793	1248960	20.0
Benzo[e]pyrene	24.790	2.9	ng	125443	6	25.101	856428	20.0
unknown26.482	26.482	2.6	ng	111855	6	25.101	856428	20.0