LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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_F\Methods\8270-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	493	496	503	rVB	25469	28148	2.58%	0.269%
2	5.422	563	567	578	rBV	1084401	923501	84.71%	8.821%
3	6.428	734	738	750	rBV	1062067	875822	80.33%	8.366%
4	6.787	795	799	802	rBV	565990	452357	41.49%	4.321%
5	7.345	889	894	897	rBV	639543	584061	53.57%	5.579%
6	8.063	1012	1016	1019	rBV	726902	572435	52.50%	5.468%
7	9.139	1195	1199	1202	rBV	1406421	1090254	100.00%	10.414%
8	9.216	1209	1212	1215	rBV5	13771	18193	1.67%	0.174%
9	9.522	1262	1264	1266	rBV	38261	31467	2.89%	0.301%
10	9.545	1266	1268	1270	rVV	30317	24714	2.27%	0.236%
11	9.575	1270	1273	1279	rVB7	18539	27966	2.57%	0.267%
12	9.680	1288	1291	1294	rBV	66724	69283	6.35%	0.662%
13	9.728	1296	1299	1302	rVB2	72467	62552	5.74%	0.597%
14	9.769	1303	1306	1308	rBV3	22701	23594	2.16%	0.225%
15	9.816	1311	1314	1318	rVV	621896	560711	51.43%	5.356%
16	9.857	1319	1321	1324	rVV3	19716	23036	2.11%	0.220%
17	9.928	1331	1333	1336	rBV3	20375	22729	2.08%	0.217%
18	9.980	1336	1342	1344	rBV2	34706	59435	5.45%	0.568%
19	10.080	1356	1359	1361	rBV2	57330	50098	4.60%	0.479%
20	10.157	1366	1372	1374	rBV4	60725	107658	9.87%	1.028%
21	10.192	1375	1378	1380	rBV3	48023	47486	4.36%	0.454%
22	10.228	1380	1384	1386	rBV2	116893	112687	10.34%	1.076%
23	10.280	1390	1393	1397	rBV5	43476	63810	5.85%	0.609%
24	10.475	1423	1426	1430	rVB2	120812	139857	12.83%	1.336%
25	10.610	1445	1449	1452	rBV	546477	506100	46.42%	4.834%
26	10.745	1469	1472	1479	rVB	485525	442751	40.61%	4.229%
27	11.210	1548	1551	1556	rVB	524796	493155	45.23%	4.711%
28	11.310	1565	1568	1570	rBV	558287	463433	42.51%	4.427%
29	11.563	1609	1611	1614	rVB	120436	89562	8.21%	0.855%
30	11.845	1657	1659	1663	rVB4	110513	106210	9.74%	1.014%
31	12.527	1772	1775	1777	rVB	106014	96989	8.90%	0.926%
32	12.757	1811	1814	1817	rVB	115920	92106	8.45%	0.880%
33	12.904	1835	1839	1842	rBV	993537	842099	77.24%	8.044%
34	13.957	2014	2018	2021	rBV	528721	563229	51.66%	5.380%
35	13.986	2021	2023	2025	rVB	59108	46963	4.31%	0.449%
36	14.439	2098	2100	2103	rVB3	24782	23580	2.16%	0.225%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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_F\Methods\8270-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.474	2103	2106	2109	rBV2	16633	16813	1.54%	0.161%
38	14.827	2163	2166	2168	rBV2	19595	18640	1.71%	0.178%
39	15.004	2192	2196	2199	rBV2	50716	74647	6.85%	0.713%
40	15.310	2244	2248	2250	rVB	31034	35541	3.26%	0.339%
41	15.368	2254	2258	2264	rVB	43804	58268	5.34%	0.557%
42	15.433	2264	2269	2274	rBV	377989	486389	44.61%	4.646%
43	15.939	2351	2355	2359	rBV6	12375	20087	1.84%	0.192%
44	16.921	2520	2522	2528	rVB3	15275	20854	1.91%	0.199%

Sum of corrected areas: 10469270

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BNA_F
ClientSampleId :
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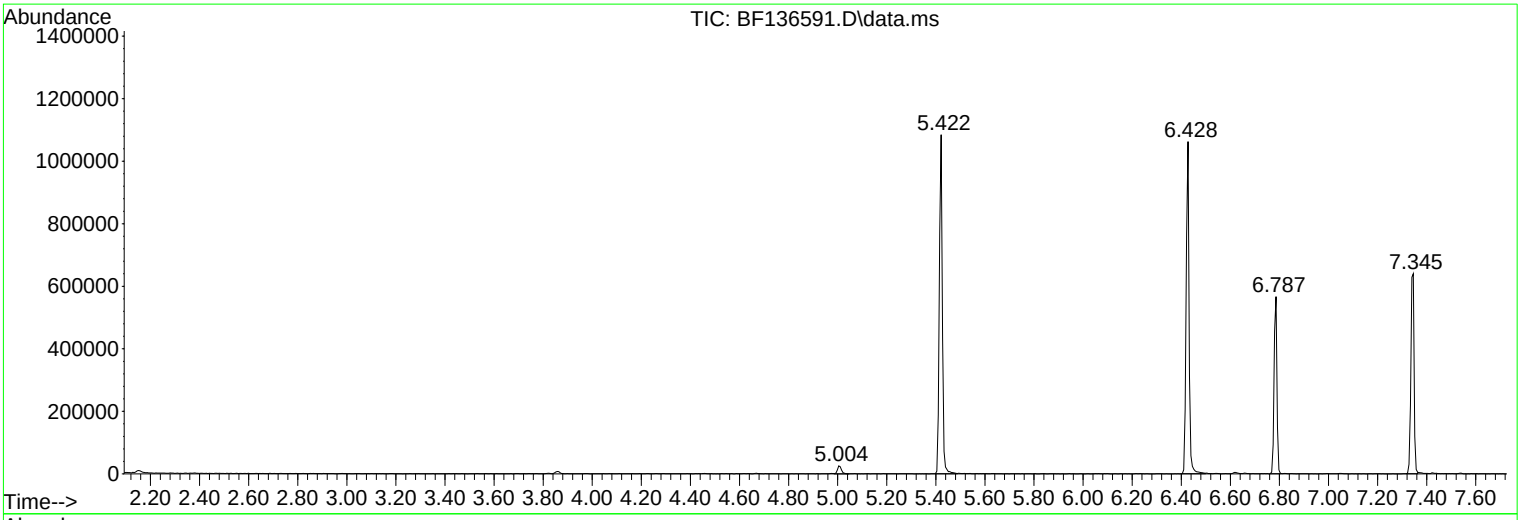
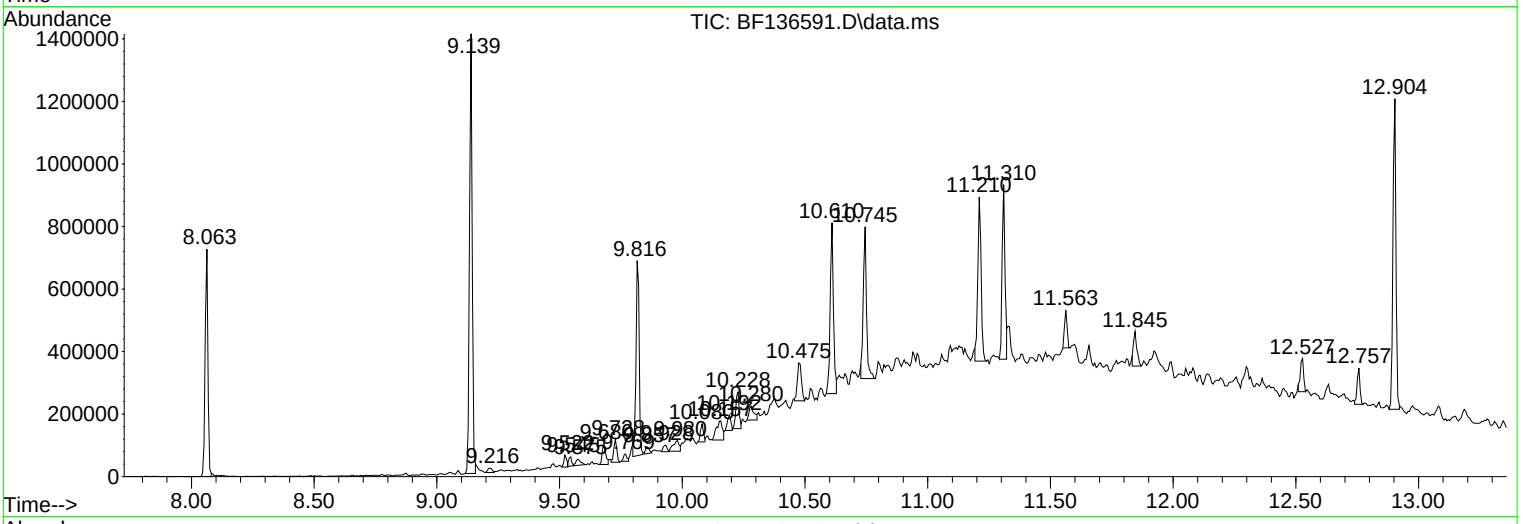
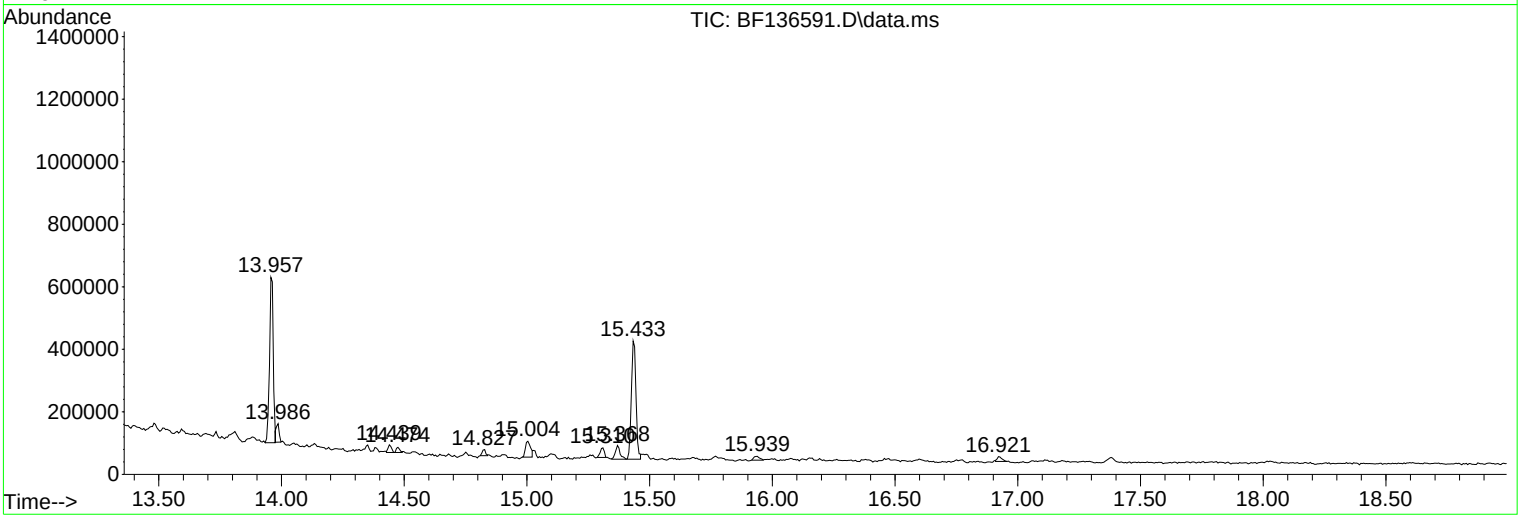
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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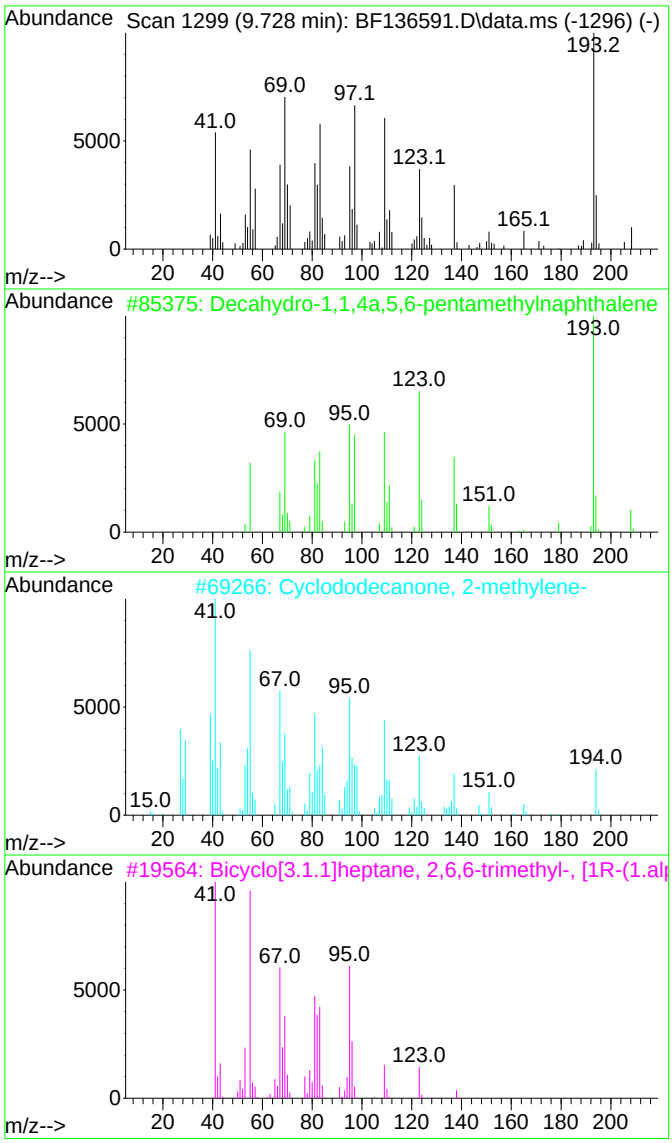
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

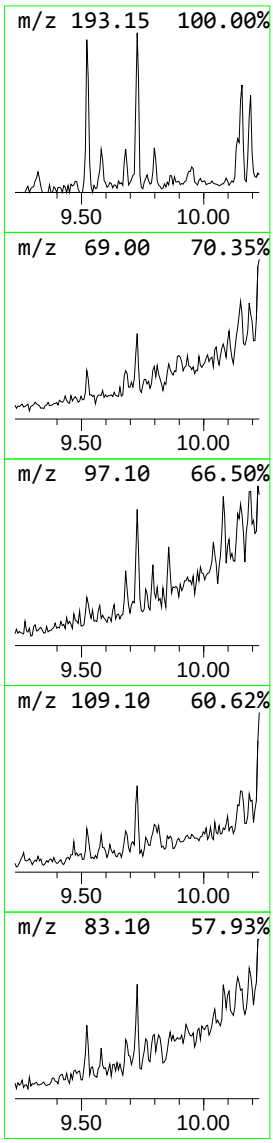
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	2.23 ng	62552	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	55
2	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	22
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	18
4	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	18
5	1a,2,5,5Tetramethyl-trans-1a,4a,...	194	C13H22O	1000215-77-6	15





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Data File : BF136591.D
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Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

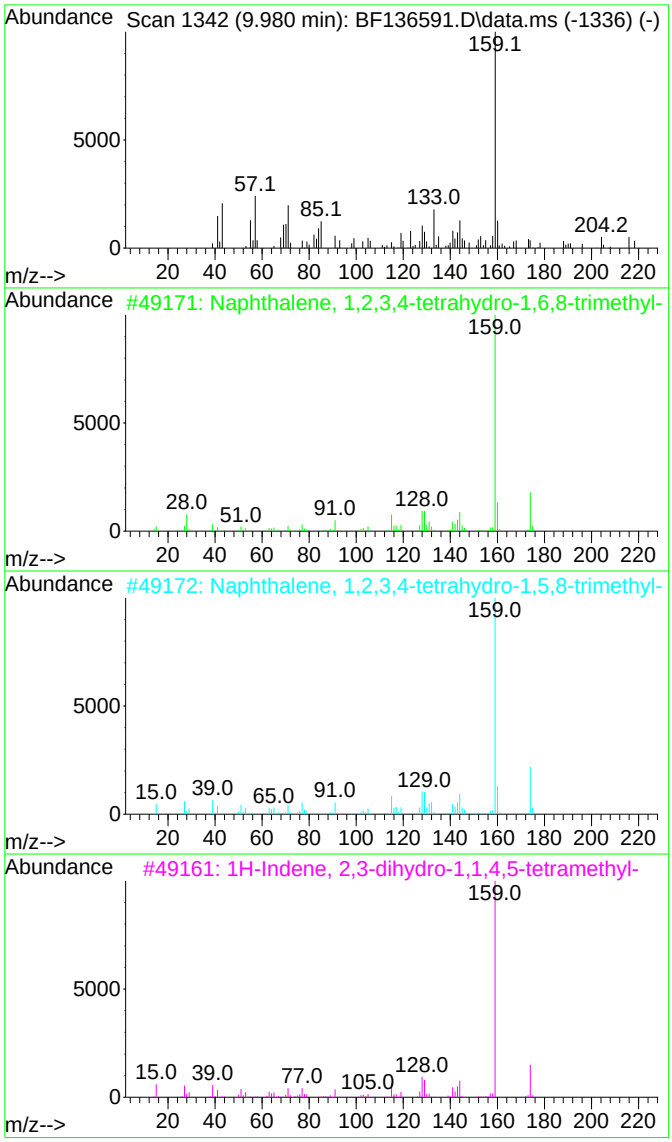
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

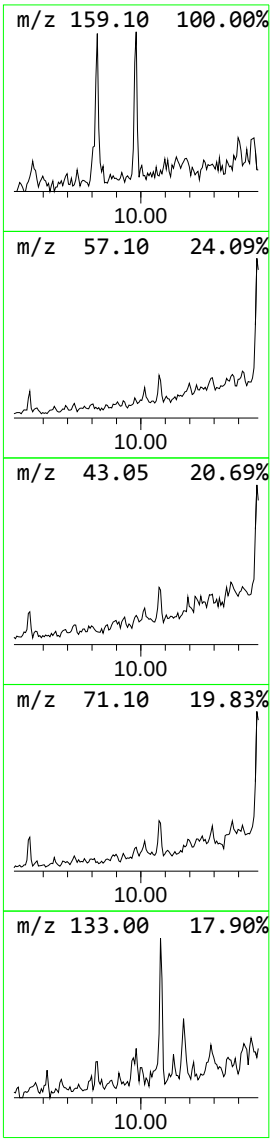
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	2.12 ng	59435	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	64
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	64
3	1H-Indene, 2,3-dihydro-1,1,4,5-t...	174	C13H18	016204-57-2	55
4	1H-Indene, 2,3-dihydro-1,1,4,7-t...	174	C13H18	001078-04-2	55
5	Indan, 1,1,6,7-tetramethyl-	174	C13H18	016204-58-3	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

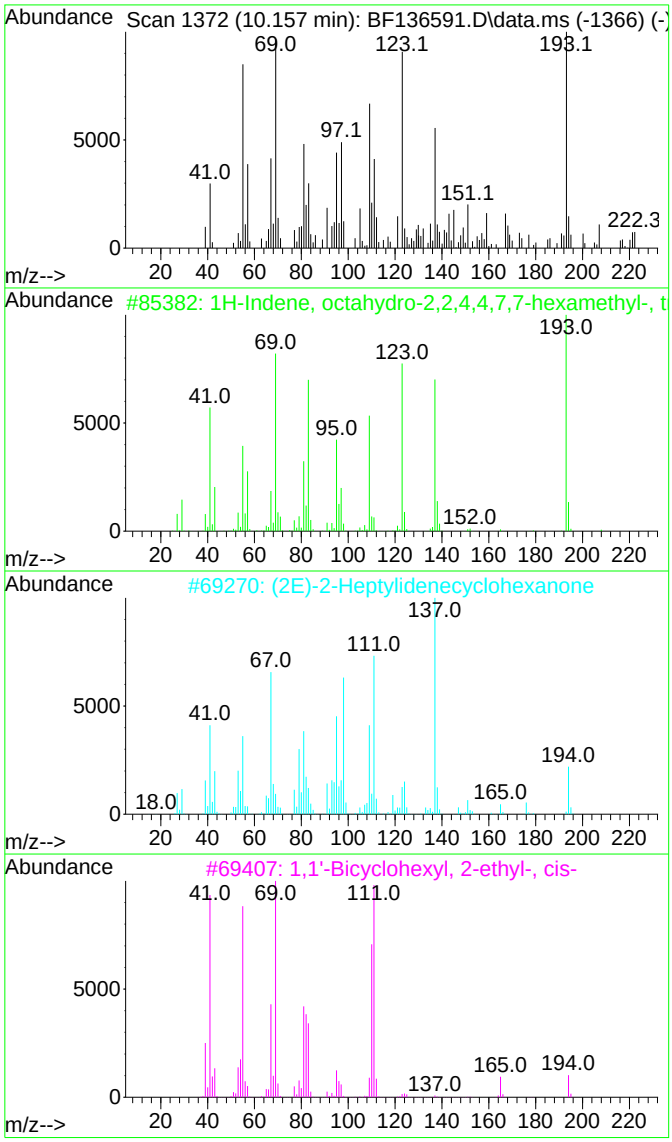
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

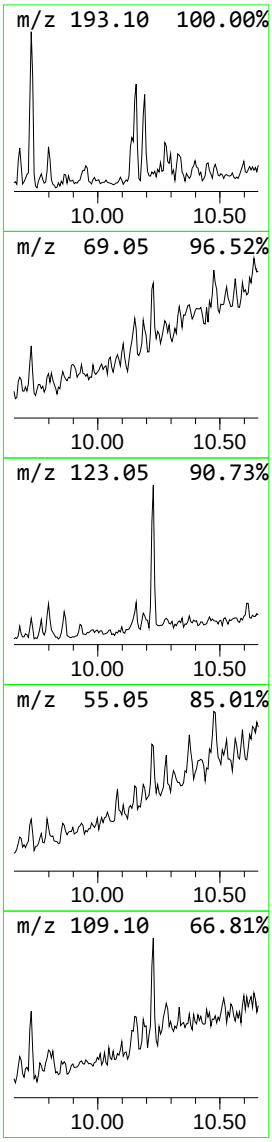
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Indene, octahydro-2,2,4,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.157	3.84 ng	107658	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	72
2	(2E)-2-Heptylidenecyclohexanone	194	C13H22O	173975-69-4	35
3	1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	15
4	2-Anthracenamine	193	C14H11N	000613-13-8	11
5	Benzoic acid, 3-fluoro-, ethyl e...	168	C9H9FO2	000451-02-5	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

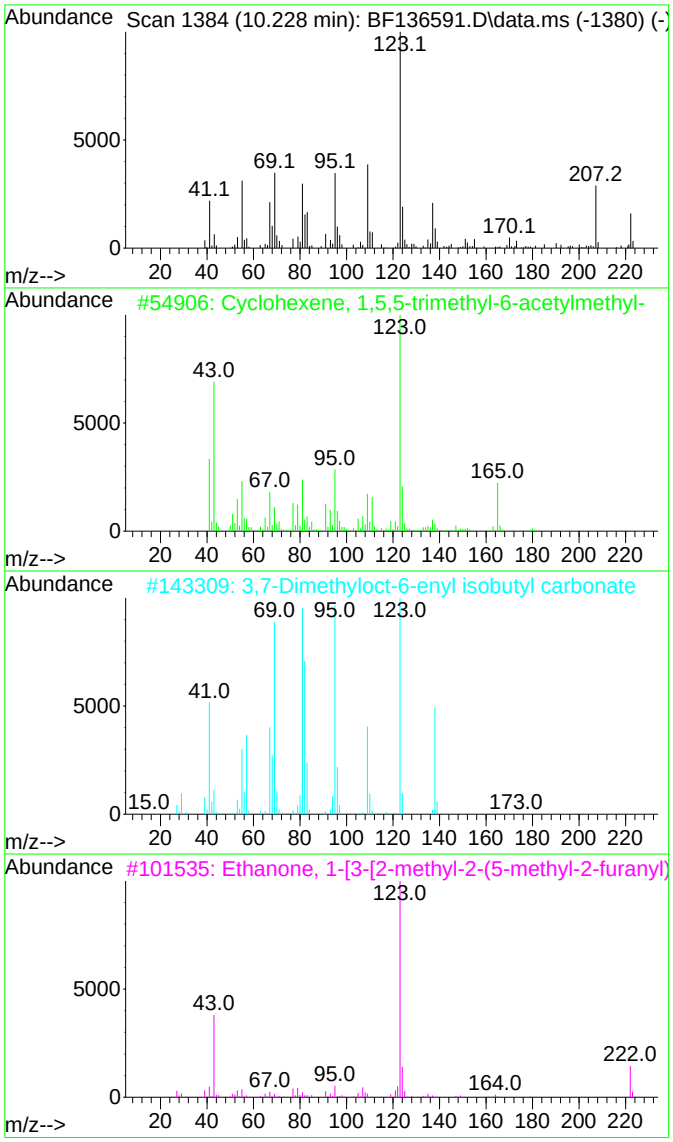
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

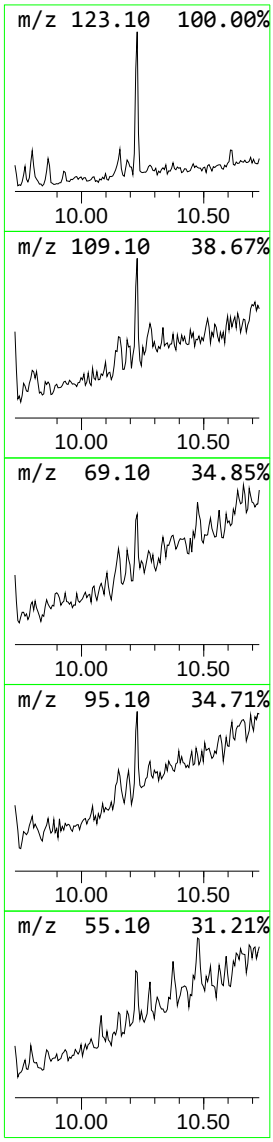
****

Peak Number 5 unknown10.227 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.227	4.02 ng	112687	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	47
2	3,7-Dimethyloct-6-enyl isobutyl ...	256	C15H28O3	1000372-79-6	43
3	Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	38
4	4-Fluorobenzoic acid, 2,2,2-trif...	222	C9H6F4O2	1000325-53-2	38
5	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

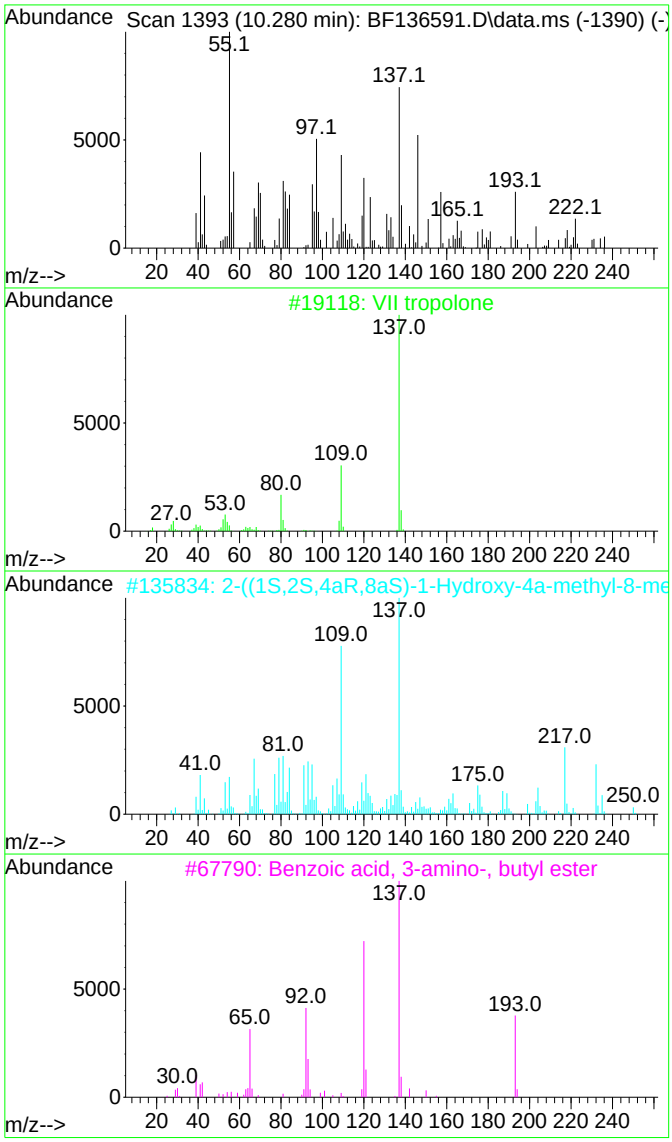
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

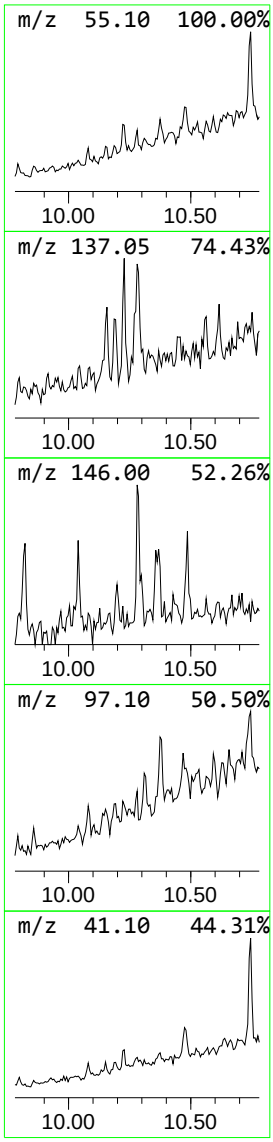
****

Peak Number 6 unknown10.281 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.281	2.28 ng	63810	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	VII tropolone	137	C7H7NO2	007021-46-7	30
2	2-((1S,2S,4aR,8aS)-1-Hydroxy-4a-...	250	C15H22O3	058728-37-3	27
3	Benzoic acid, 3-amino-, butyl ester	193	C11H15NO2	1000374-53-9	27
4	1-(2-Hydroxy-6-(isopentyloxy)phe...	222	C13H18O3	1010297-97-1	18
5	2(1H)-Pyridone, 1-ethyl-4-methyl-	137	C8H11NO	019006-62-3	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

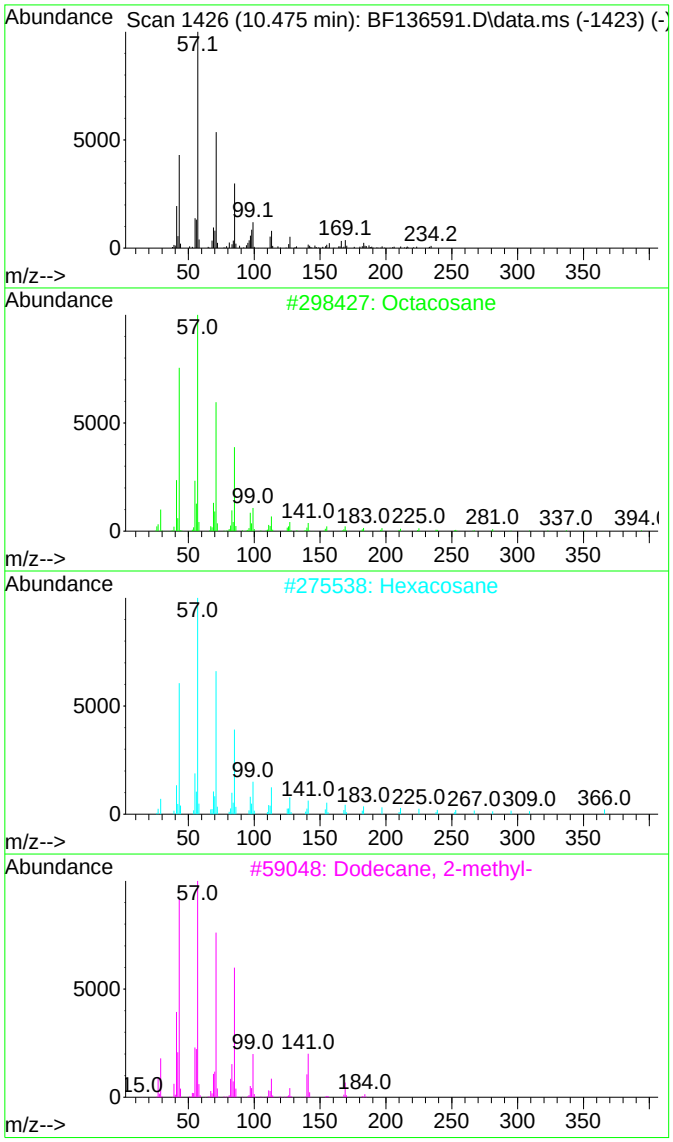
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

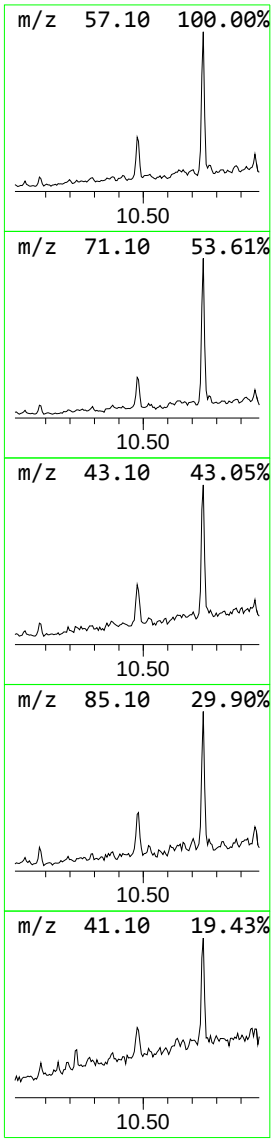
****

Peak Number 7 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	4.99 ng	139857	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	80
2	Hexacosane	366	C26H54	000630-01-3	72
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
4	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	64
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	64





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Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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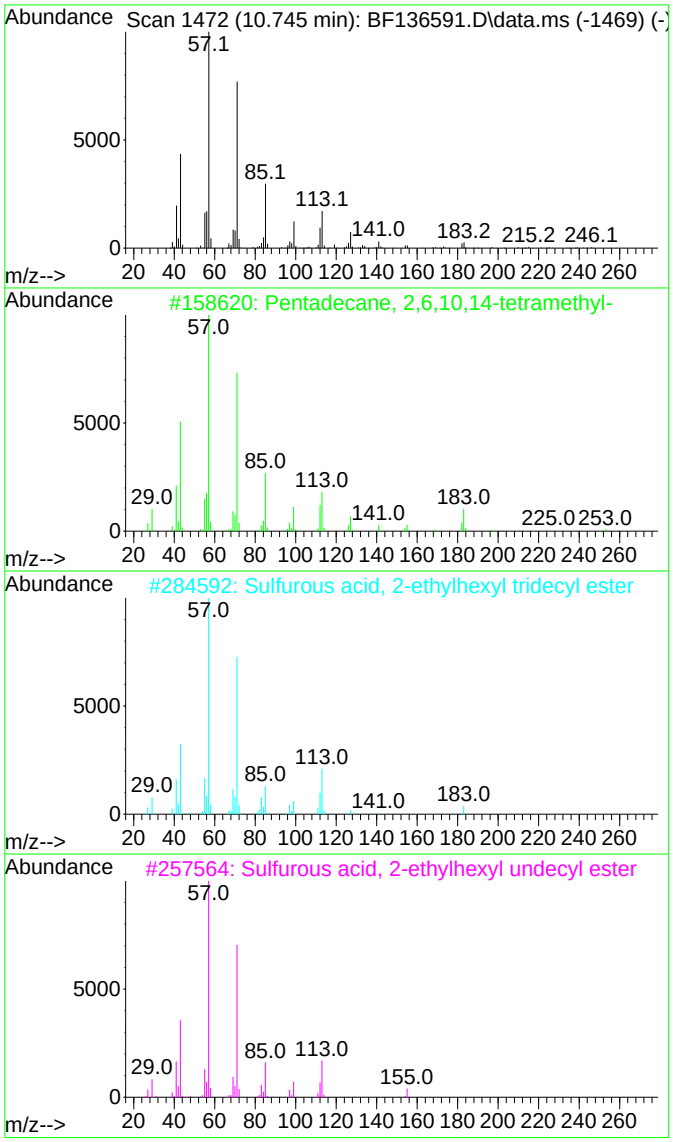
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

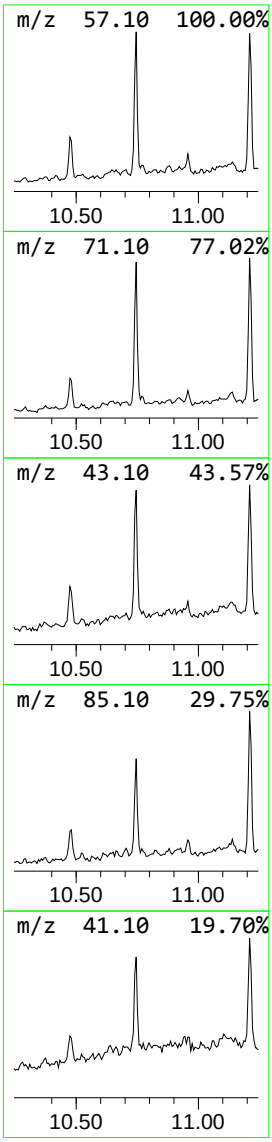
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentadecane, 2,6,10,14-tetr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	19.11 ng	442751	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	86
3	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	86
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	81
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

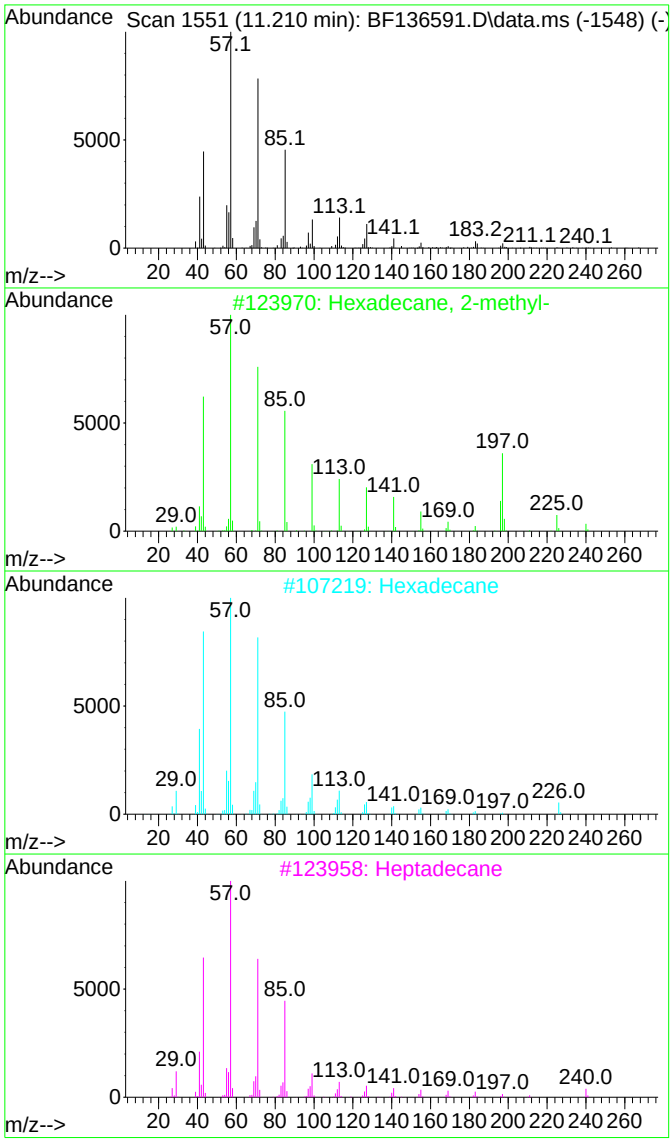
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

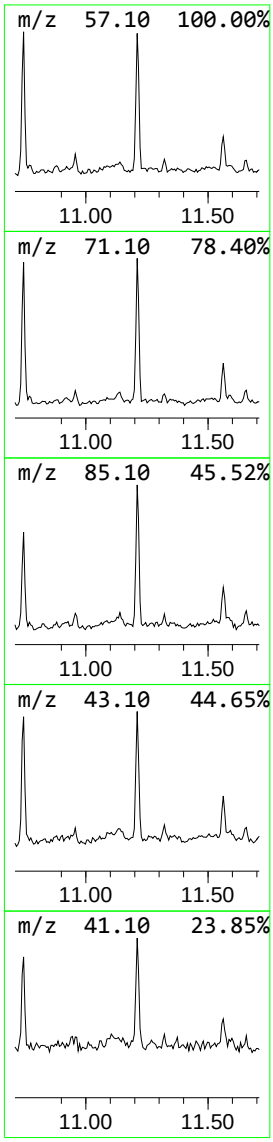
****

Peak Number 9 Hexadecane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.210	21.28 ng	493155	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5	Octadecane	254	C18H38	000593-45-3	90





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Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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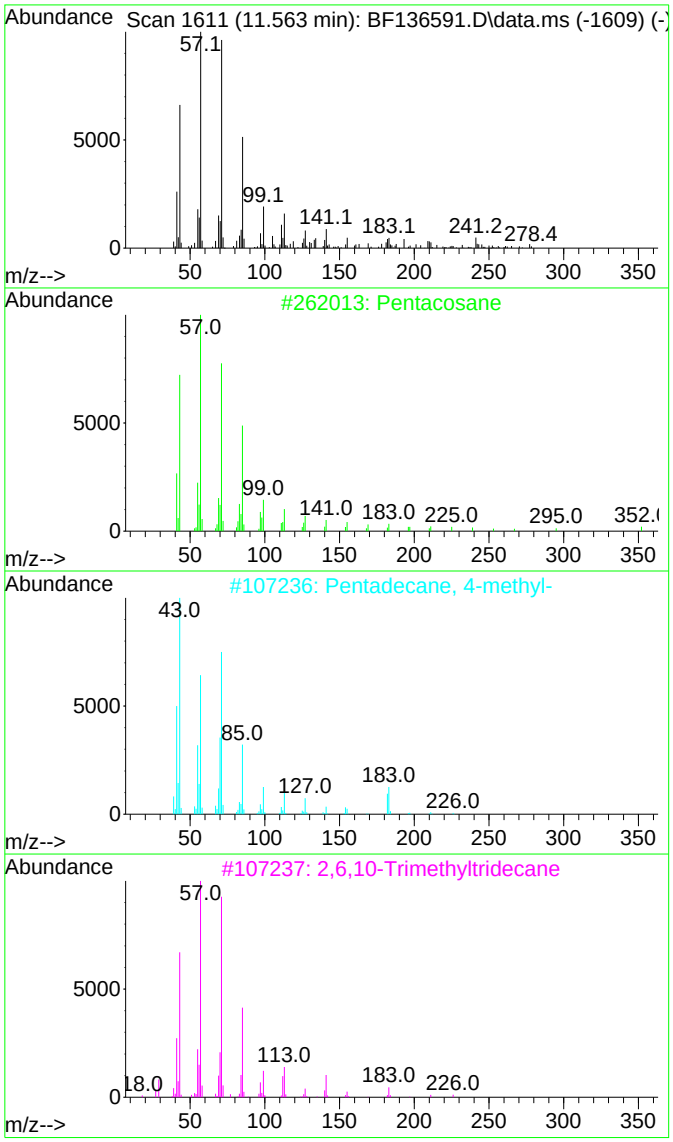
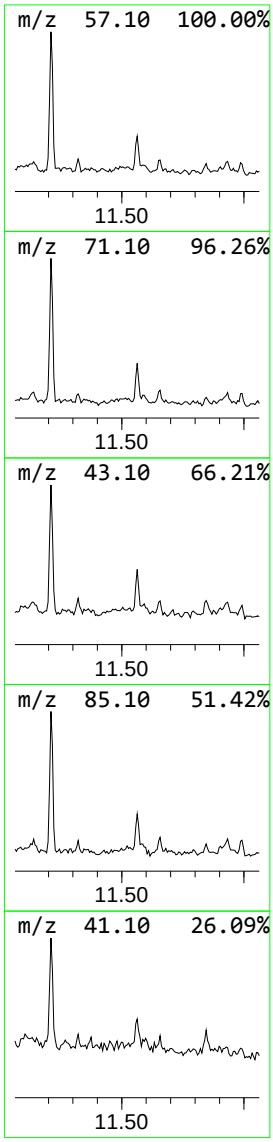
Peak Number 10 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.563	3.87 ng	89562	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	87
3	2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	86
4	Octadecane	254	C18H38	000593-45-3	86
5	1,3-Propanediol, ethyl tetradecy...	300	C19H40O2	1000406-35-2	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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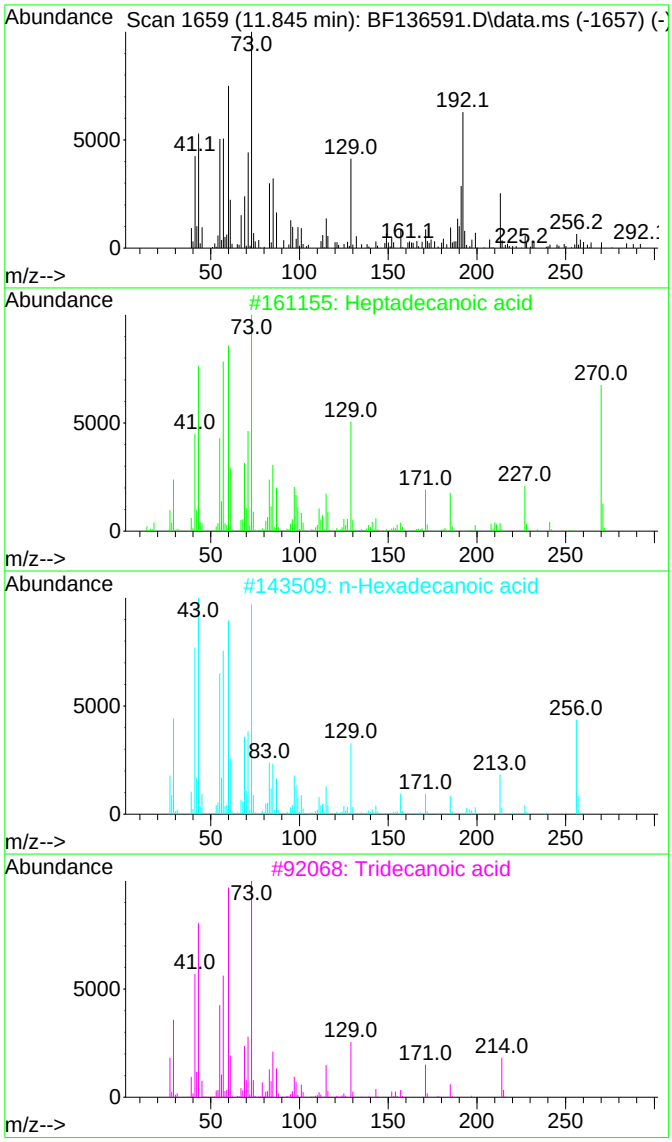
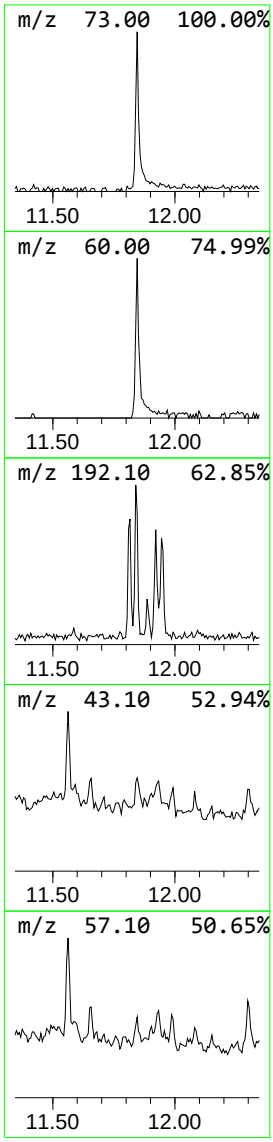
Peak Number 11 Heptadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	4.58 ng	106210	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid	270	C17H34O2	000506-12-7	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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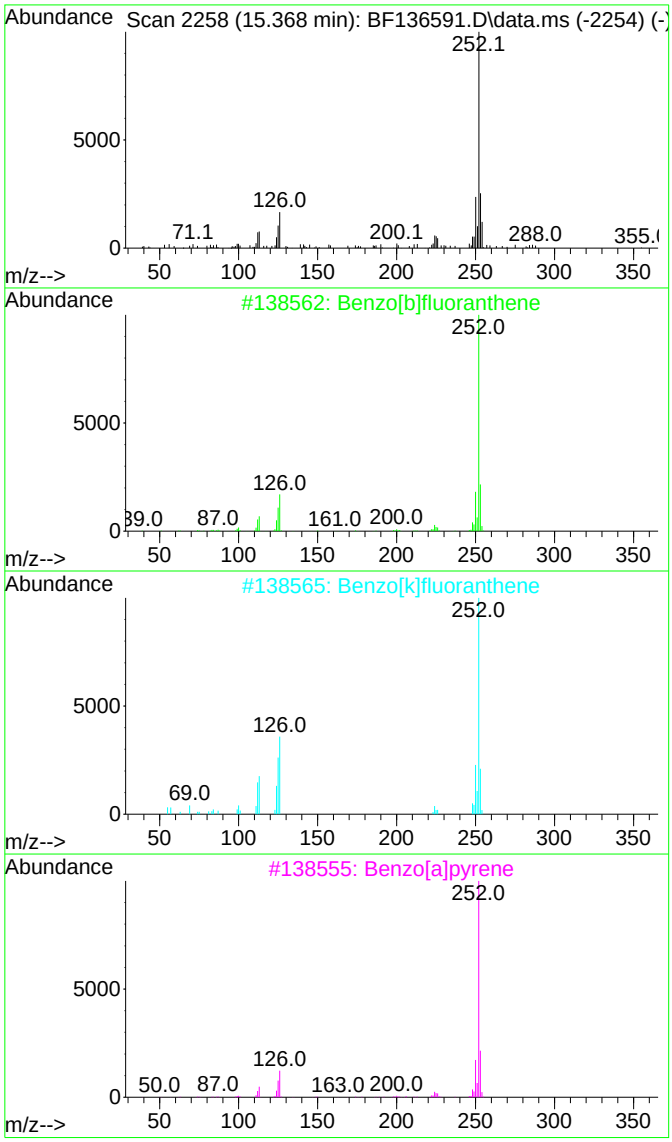
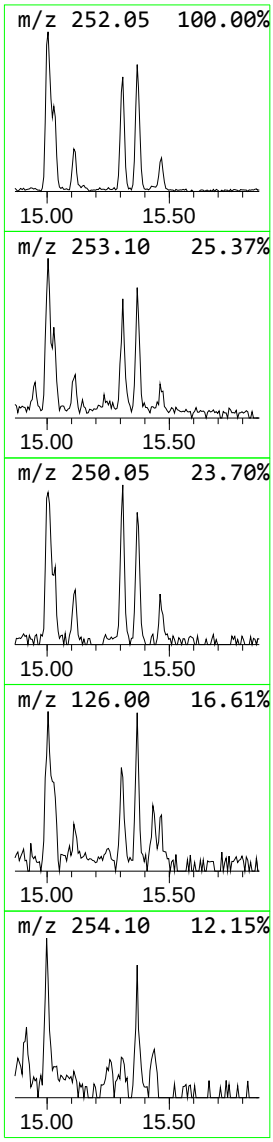
Peak Number 12 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	2.40 ng	58268	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	94
4	Benzo[e]pyrene	252	C20H12	000192-97-2	94
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121523\
Data File : BF136591.D
Acq On : 15 Dec 2023 14:17
Operator : CG\JU
Sample : 05769-01 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
Decahydro-1,1,4...	9.728	2.2	ng	62552	3	9.816	560711	20.0
Naphthalene, 1,...	9.980	2.1	ng	59435	3	9.816	560711	20.0
1H-Indene, octa...	10.157	3.8	ng	107658	3	9.816	560711	20.0
unknown10.227	10.227	4.0	ng	112687	3	9.816	560711	20.0
unknown10.281	10.281	2.3	ng	63810	3	9.816	560711	20.0
Octacosane	10.475	5.0	ng	139857	3	9.816	560711	20.0
Pentadecane, 2,...	10.745	19.1	ng	442751	4	11.310	463433	20.0
Hexadecane, 2-m...	11.210	21.3	ng	493155	4	11.310	463433	20.0
Pentacosane	11.563	3.9	ng	89562	4	11.310	463433	20.0
Heptadecanoic acid	11.845	4.6	ng	106210	4	11.310	463433	20.0
Benzo[e]pyrene	15.368	2.4	ng	58268	6	15.433	486389	20.0