LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-346

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.351	179	181	192	rBV	35864	69340	3.11%	0.438%
2	5.040	465	468	473	rVB	27377	31059	1.39%	0.196%
3	5.469	538	541	550	rBV	2104807	2099167	94.18%	13.273%
4	6.481	710	713	724	rVB	2110734	2109861	94.65%	13.340%
5	6.563	724	727	730	rVB	44614	28578	1.28%	0.181%
6	6.822	767	771	774	rBV	618204	463629	20.80%	2.931%
7	7.386	862	867	870	rBV	1603145	1410783	63.29%	8.920%
8	8.104	985	989	992	rBV	696616	548283	24.60%	3.467%
9	9.186	1167	1173	1176	rBV	2382597	2229006	100.00%	14.094%
10	9.863	1284	1288	1291	rBV	621261	519661	23.31%	3.286%
11	10.651	1418	1422	1426	rBV	1414123	1186444	53.23%	7.502%
12	11.345	1537	1540	1543	rBV	517533	464067	20.82%	2.934%
13	11.369	1543	1544	1548	rVB	87973	59491	2.67%	0.376%
14	11.745	1605	1608	1611	rBV	72747	59964	2.69%	0.379%
15	11.880	1628	1631	1637	rBV	188316	160484	7.20%	1.015%
16	11.963	1641	1645	1647	rBV2	23877	24635	1.11%	0.156%
17	12.451	1722	1728	1731	rBV3	81613	76574	3.44%	0.484%
18	12.563	1744	1747	1750	rBV	145302	124727	5.60%	0.789%
19	12.663	1760	1764	1771	rBV4	53390	72891	3.27%	0.461%
20	12.792	1780	1786	1789	rBV	131769	130188	5.84%	0.823%
21	12.939	1807	1811	1814	rBV	2158343	1806472	81.04%	11.422%
22	13.627	1923	1928	1933	rBV2	18618	29186	1.31%	0.185%
23	13.739	1942	1947	1950	rBV3	17472	28314	1.27%	0.179%
24	13.845	1960	1965	1966	rBV3	41747	49050	2.20%	0.310%
25	13.992	1985	1990	1993	rBV	567419	560405	25.14%	3.543%
26	14.015	1993	1994	2000	rVB	83305	59179	2.65%	0.374%
27	14.092	2001	2007	2012	rBV	173169	201520	9.04%	1.274%
28	14.157	2016	2018	2022	rVB	23298	23263	1.04%	0.147%
29	14.468	2068	2071	2074	rBV2	38591	38768	1.74%	0.245%
30	14.627	2095	2098	2102	rVB3	27784	28123	1.26%	0.178%
31	14.774	2119	2123	2126	rVB	40193	42566	1.91%	0.269%
32	15.027	2162	2166	2176	rVB	71190	134330	6.03%	0.849%
33	15.109	2177	2180	2184	rBV	42689	48176	2.16%	0.305%
34	15.327	2214	2217	2224	rVB	36420	52426	2.35%	0.331%
35	15.392	2224	2228	2233	rBV	52617	65016	2.92%	0.411%
36	15.457	2234	2239	2243	rVV	326503	418743	18.79%	2.648%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
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Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.492	2243	2245	2251	rVB2	59174	68031	3.05%	0.430%
38	15.927	2314	2319	2327	rVB	54439	78528	3.52%	0.497%
39	16.433	2398	2405	2409	rBV3	39266	76623	3.44%	0.484%
40	16.898	2481	2484	2491	rVB4	18978	33039	1.48%	0.209%
41	17.021	2502	2505	2510	rVB5	23259	40006	1.79%	0.253%
42	17.333	2556	2558	2564	rVB3	17359	30542	1.37%	0.193%
43	17.727	2620	2625	2630	rVB4	16582	34329	1.54%	0.217%

Sum of corrected areas: 15815467

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
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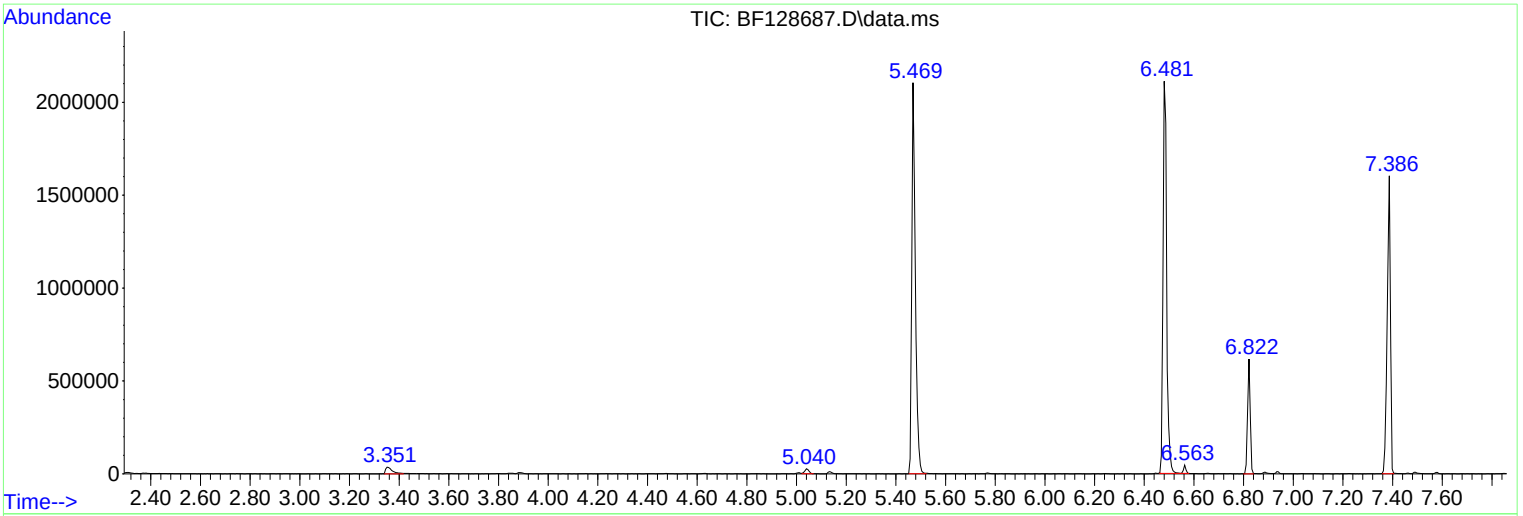
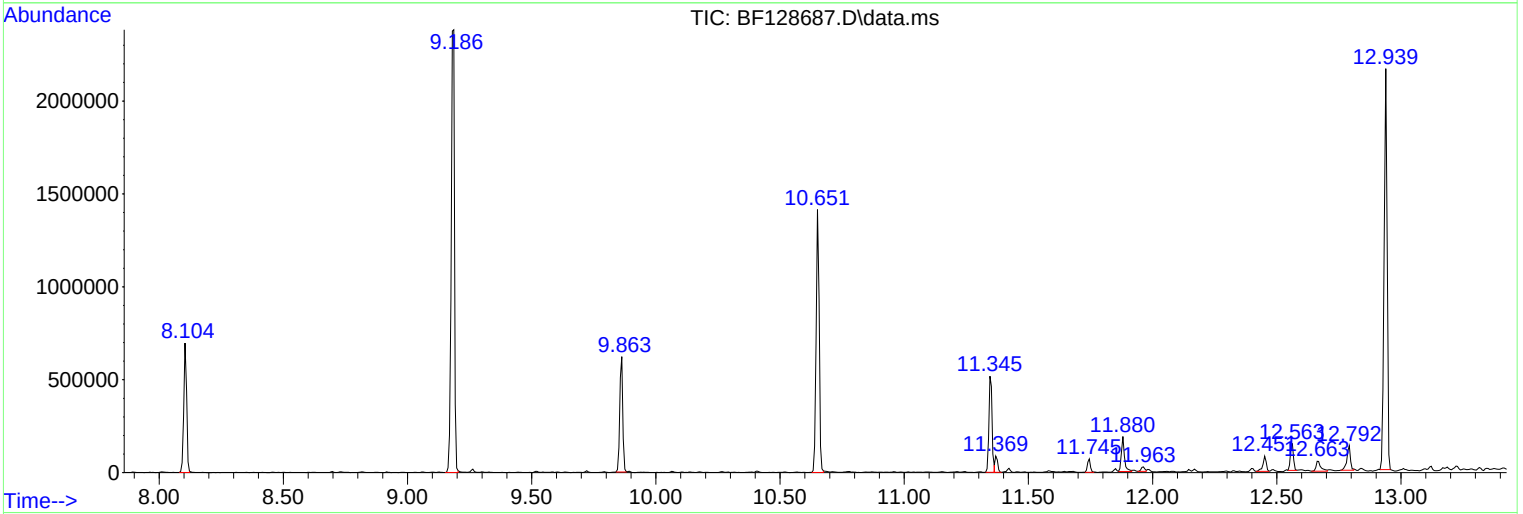
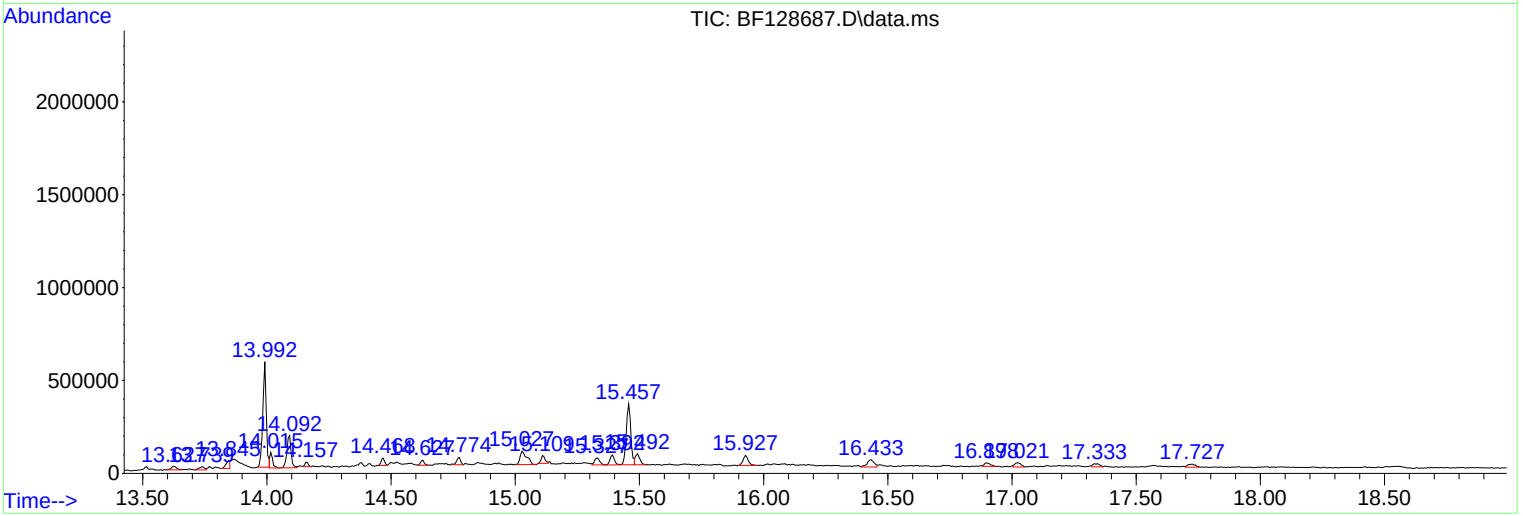
Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

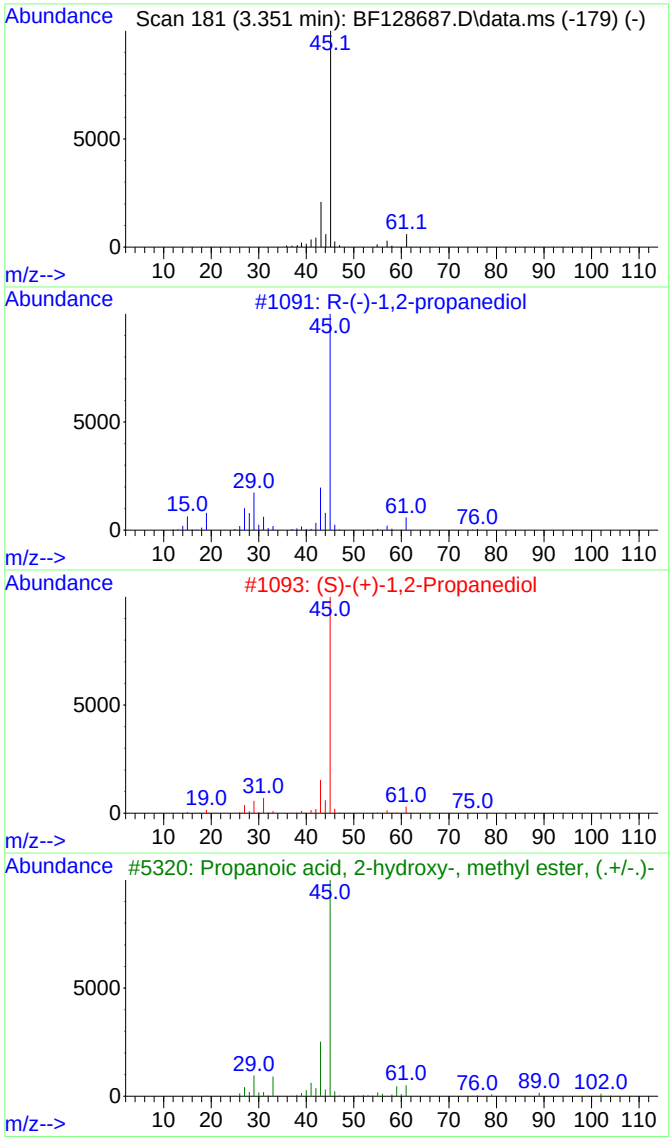
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

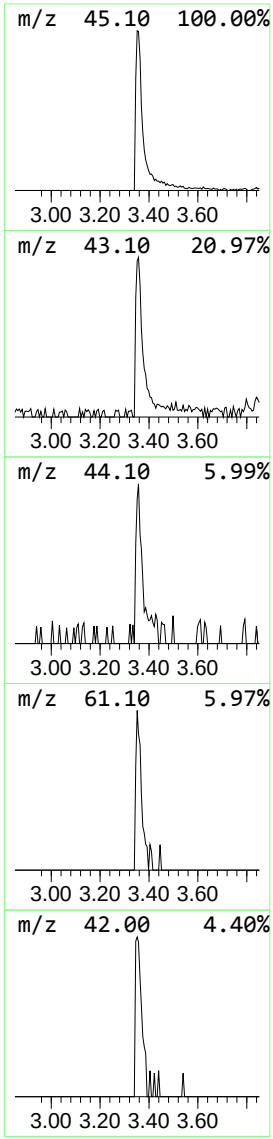
****

Peak Number 1 unknown3.351 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.351	2.99 ng	69340	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

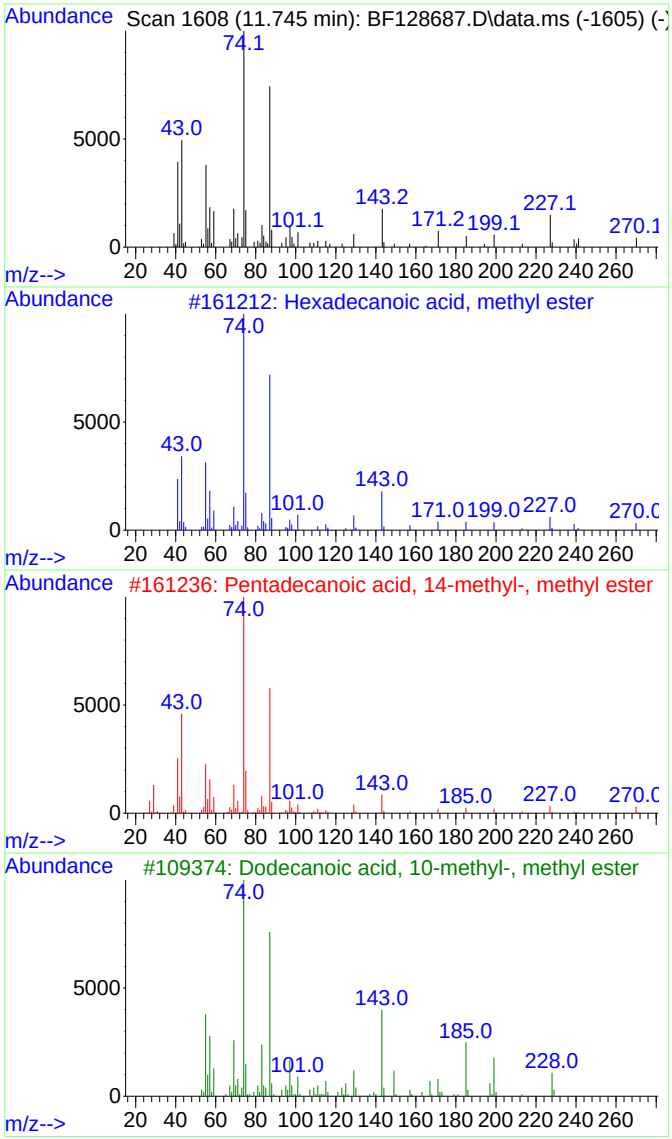
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

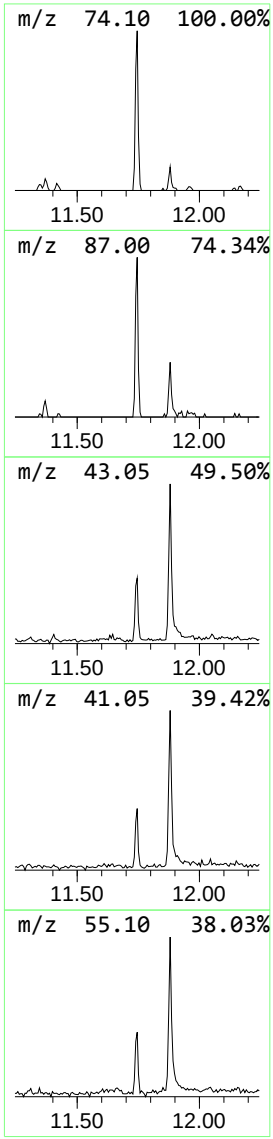
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	2.58 ng	59964	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
3	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	83
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

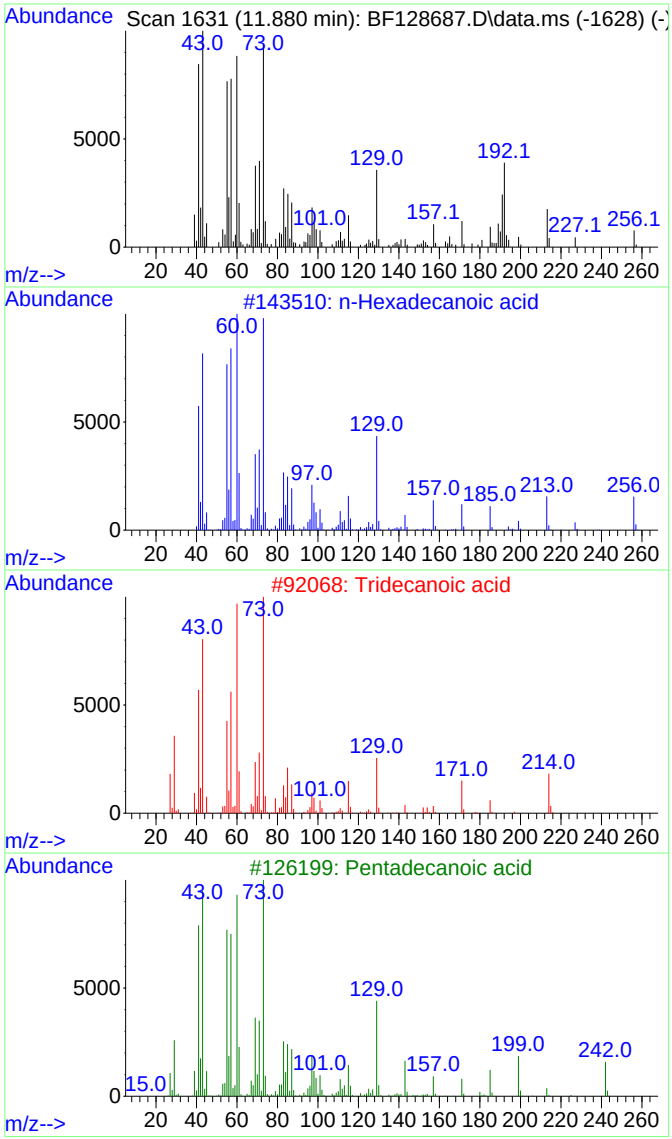
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

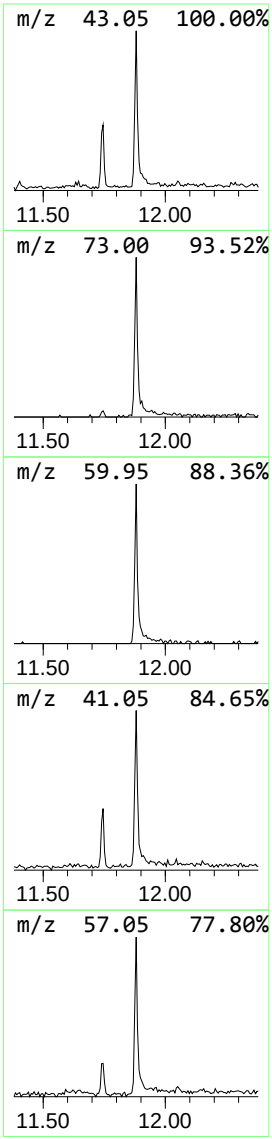
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	6.92 ng	160484	Phenanthrene-d10	11.345

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

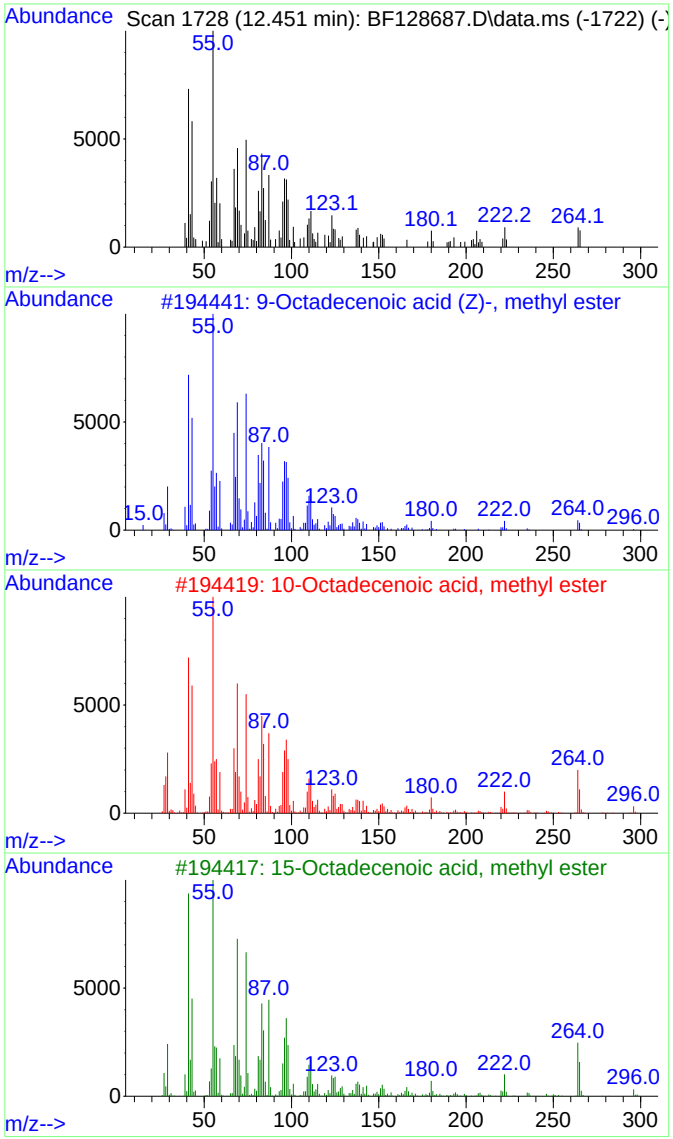
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

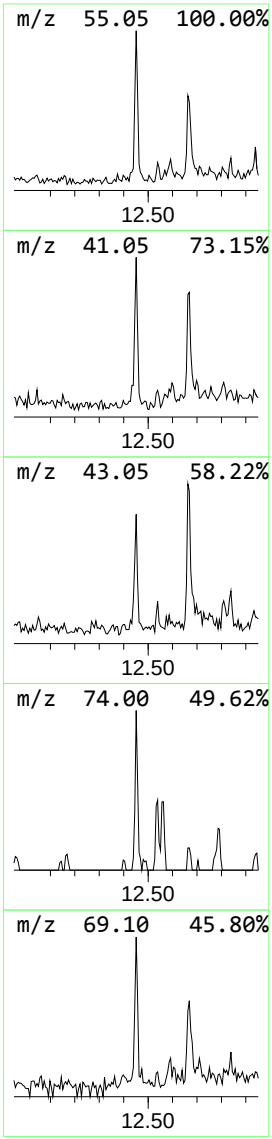
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	3.30 ng	76574	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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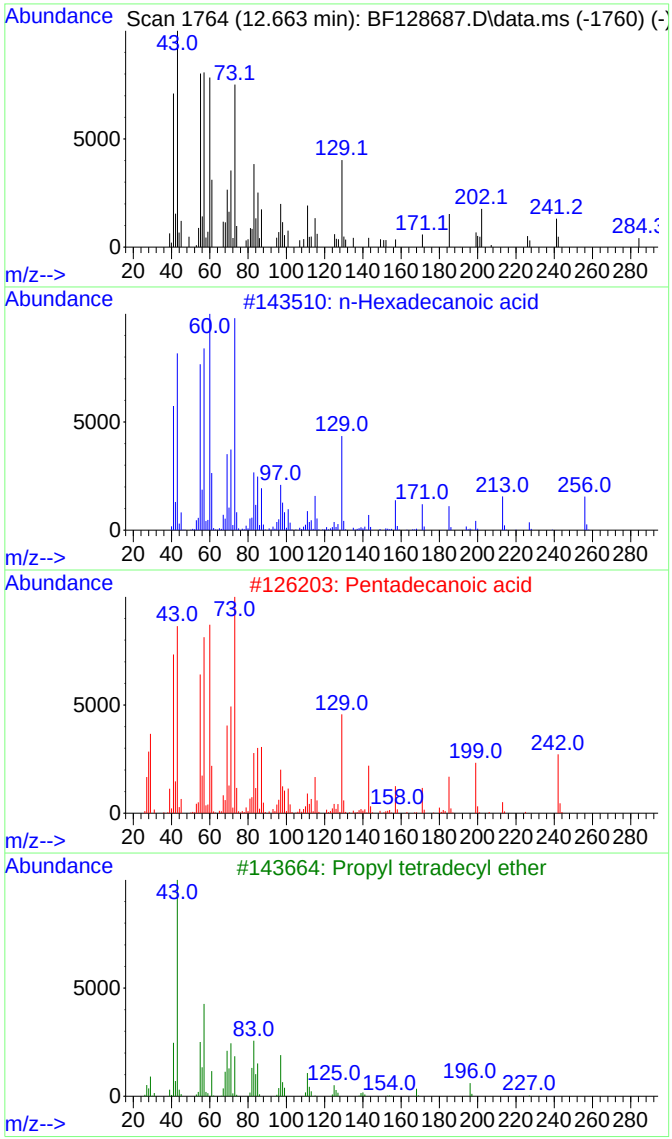
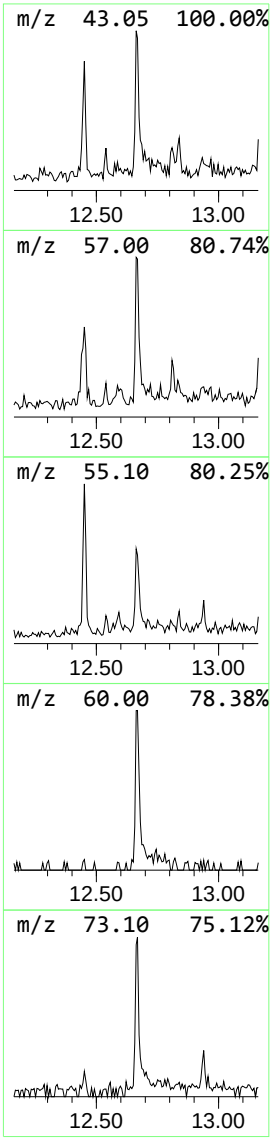
Peak Number 5 unknown12.663 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	3.14 ng	72891	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
3	Propyl tetradecyl ether	256	C17H36O	1010406-27-8	25
4	Isoamyl nitrite	117	C5H11NO2	000110-46-3	14
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	14





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Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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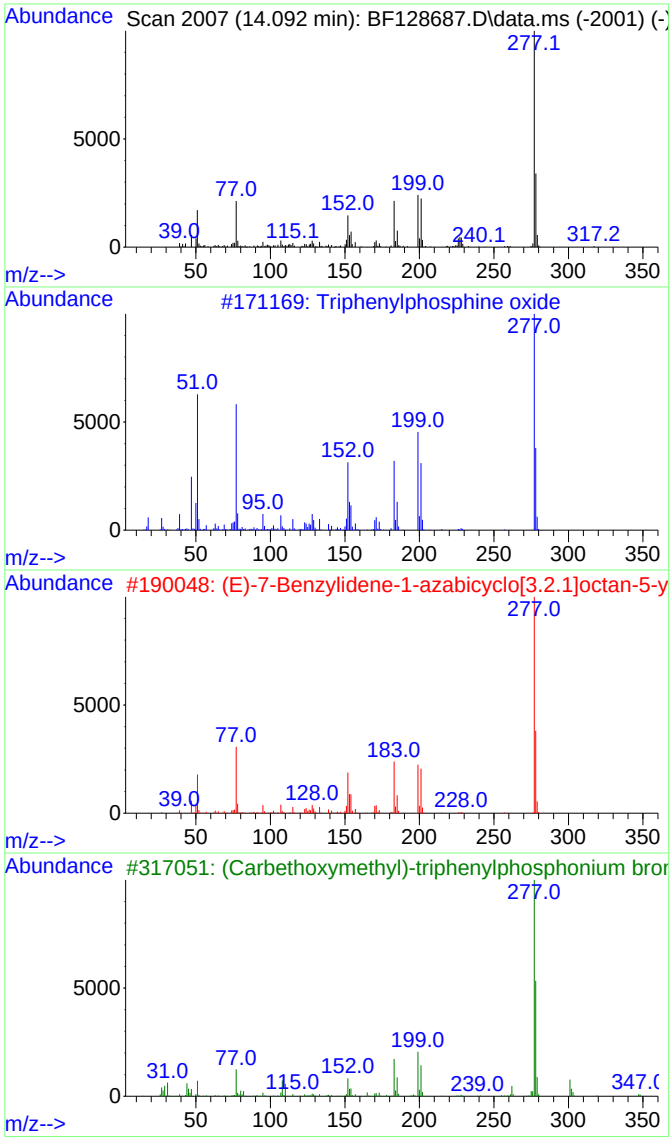
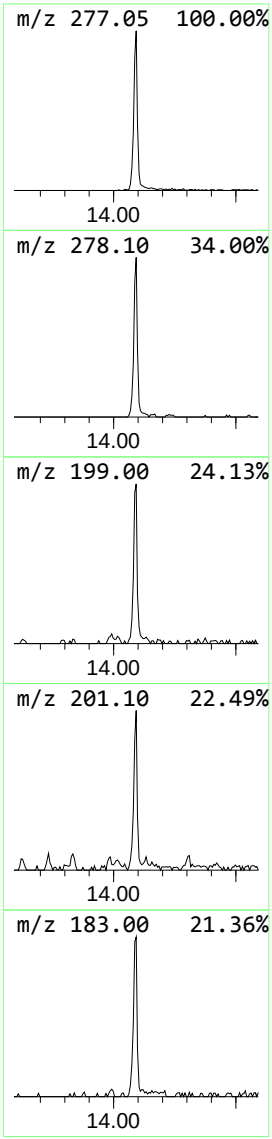
Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	7.19 ng	201520	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	99
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	70
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	38
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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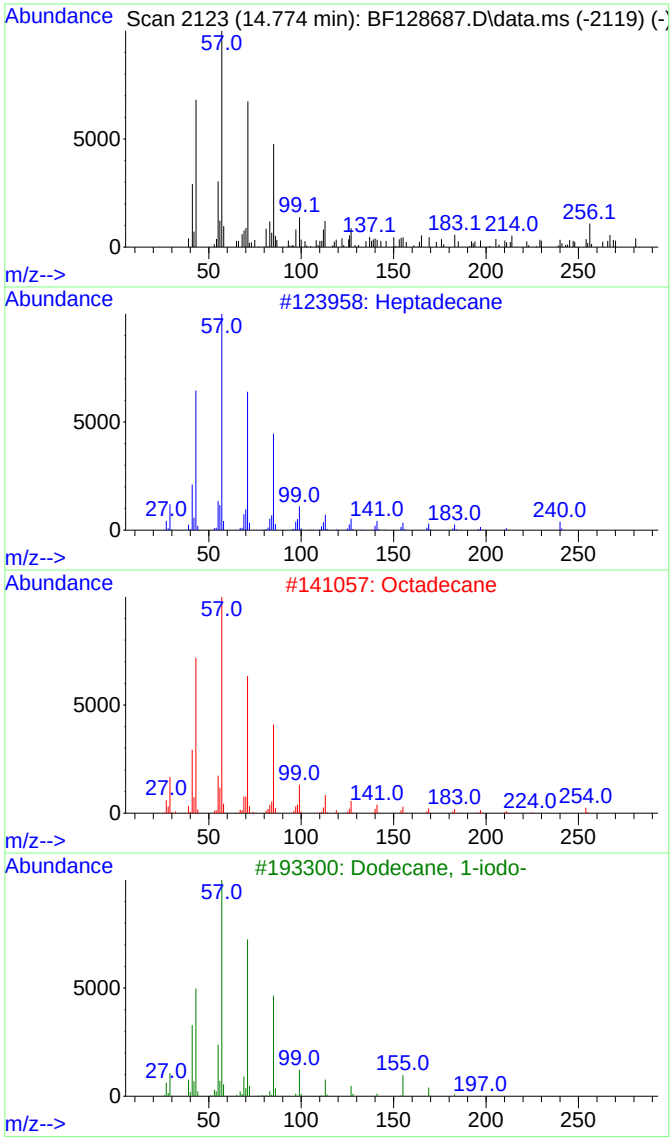
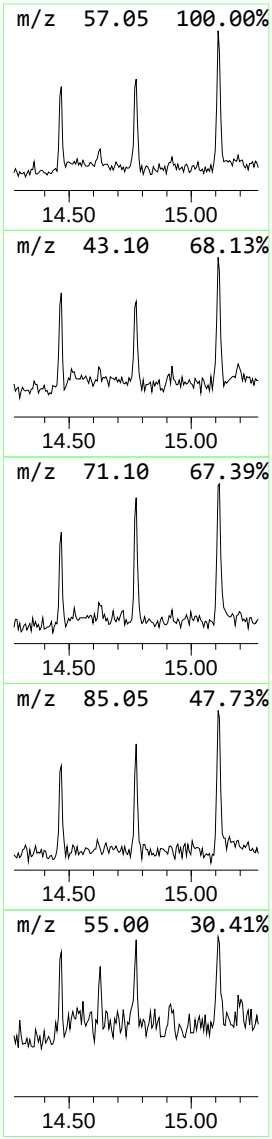
Peak Number 7 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	2.03 ng	42566	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Octadecane	254	C18H38	000593-45-3	76
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58
4	Docosane	310	C22H46	000629-97-0	58
5	Tetracosane	338	C24H50	000646-31-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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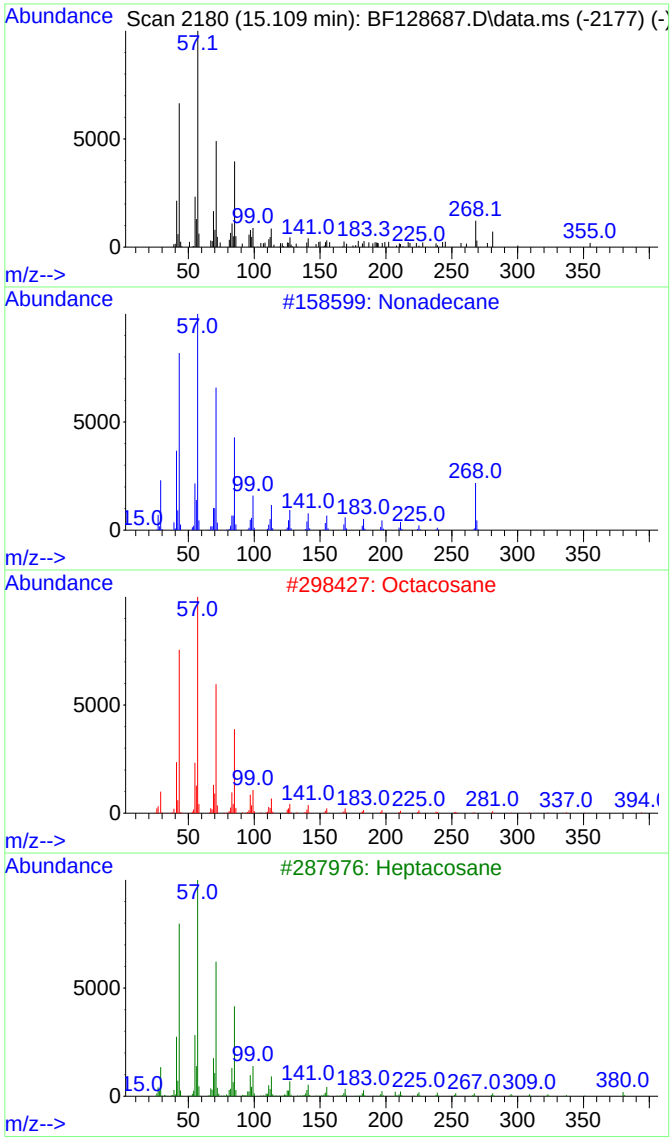
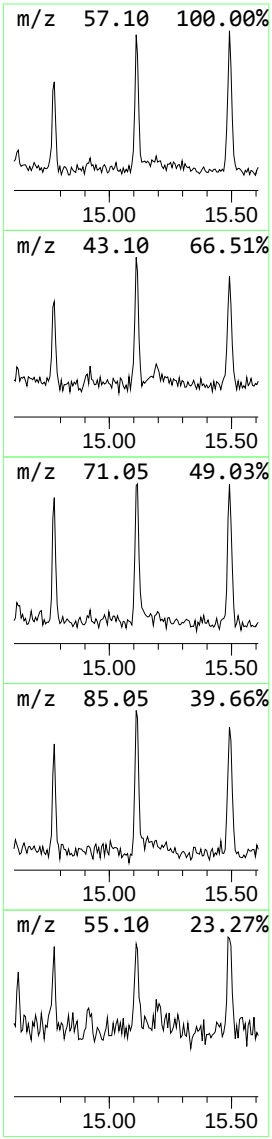
Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	2.30 ng	48176	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Octacosane	394	C28H58	000630-02-4	76
3	Heptacosane	380	C27H56	000593-49-7	70
4	Hexacosane	366	C26H54	000630-01-3	70
5	Heptadecane	240	C17H36	000629-78-7	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
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Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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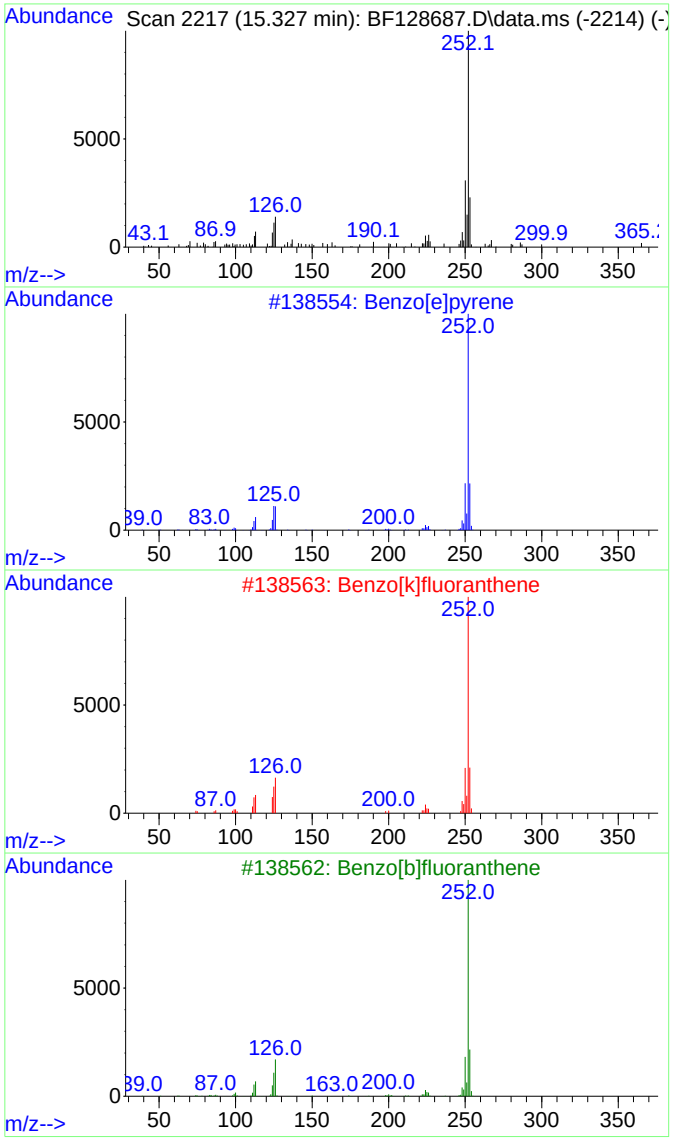
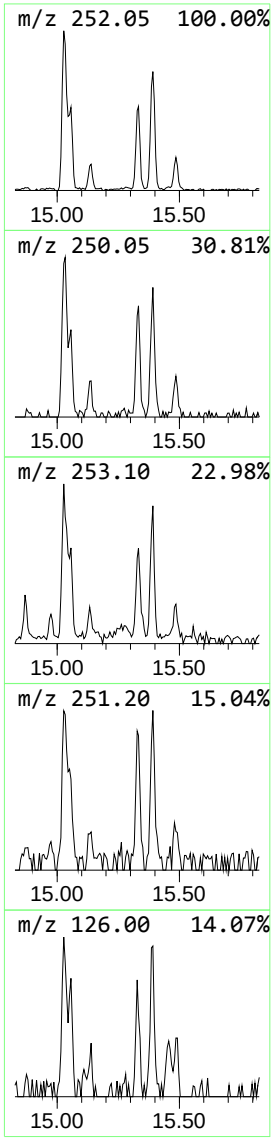
Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	2.50 ng	52426	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	90
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	76





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Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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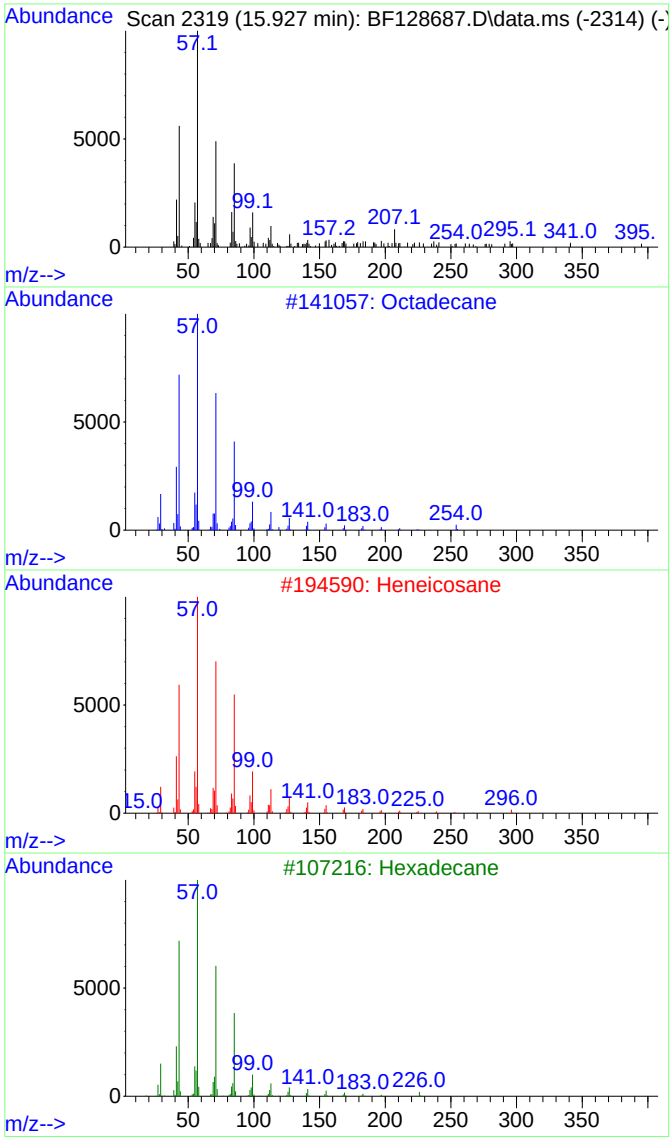
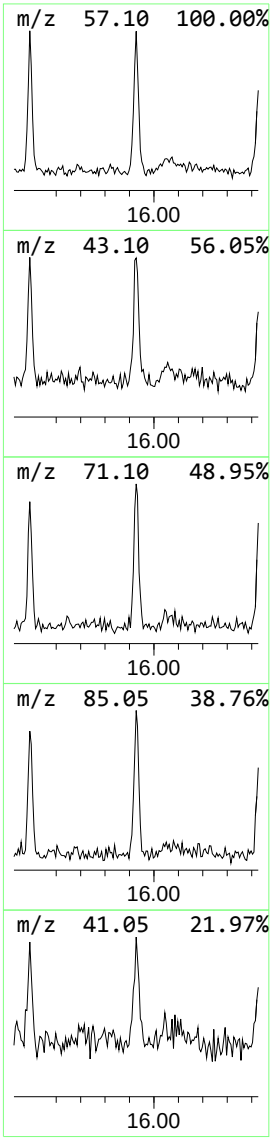
Peak Number 10 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	3.75 ng	78528	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Heneicosane	296	C21H44	000629-94-7	95
3	Hexadecane	226	C16H34	000544-76-3	95
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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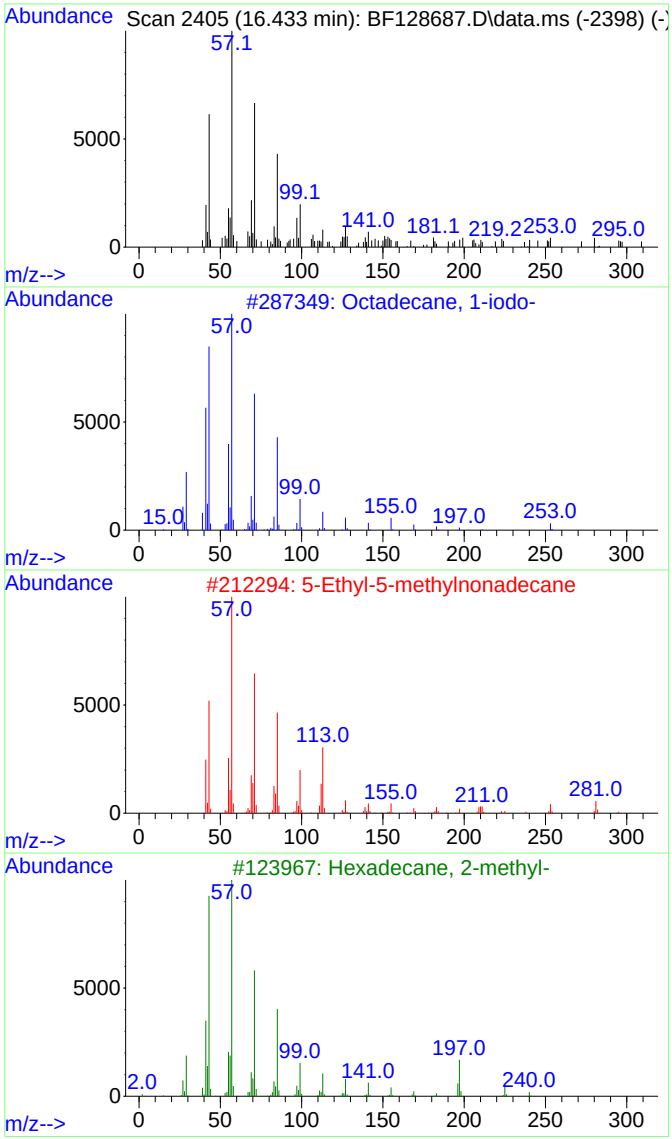
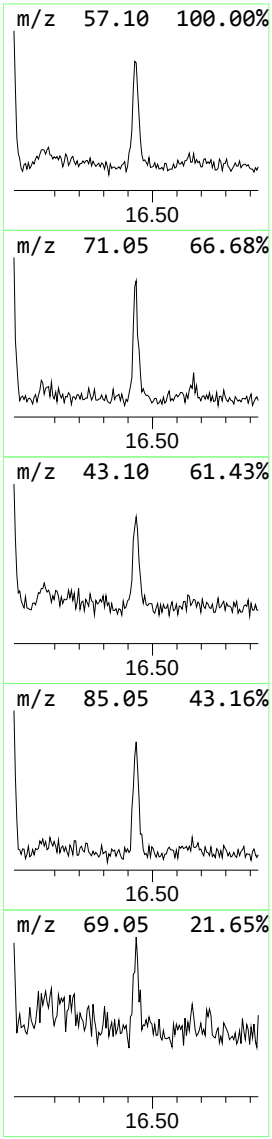
Peak Number 11 Octadecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.433	3.66 ng	76623	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
2	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	80
4	Heneicosane	296	C21H44	000629-94-7	80
5	Heptadecane	240	C17H36	000629-78-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128687.D
Acq On : 03 Jun 2022 19:09
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
unknown3.351	3.351	3.0	ng	69340	1	6.822	463629	20.0
Hexadecanoic ac...	11.745	2.6	ng	59964	4	11.345	464067	20.0
n-Hexadecanoic ...	11.880	6.9	ng	160484	4	11.345	464067	20.0
9-Octadecenoic ...	12.451	3.3	ng	76574	4	11.345	464067	20.0
unknown12.663	12.663	3.1	ng	72891	4	11.345	464067	20.0
Triphenylphosph...	14.092	7.2	ng	201520	5	13.992	560405	20.0
Heptadecane	14.774	2.0	ng	42566	6	15.457	418743	20.0
Nonadecane	15.110	2.3	ng	48176	6	15.457	418743	20.0
Benzo[e]pyrene	15.327	2.5	ng	52426	6	15.457	418743	20.0
Octadecane	15.927	3.8	ng	78528	6	15.457	418743	20.0
Octadecane, 1-i...	16.433	3.7	ng	76623	6	15.457	418743	20.0