LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128582.D
Acq On : 29 May 2022 20:30
Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS002-0006-01

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128582.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.052	467	470	475	rVB2	21014	27971	1.14%	0.176%
2	5.451	534	538	542	rBV	1953884	1853332	75.60%	11.666%
3	6.463	705	710	713	rBV	1936182	1707079	69.63%	10.745%
4	6.840	770	774	777	rBV	731999	573390	23.39%	3.609%
5	7.398	865	869	872	rBV	1425746	1134176	46.26%	7.139%
6	8.122	988	992	995	rBV	791090	633974	25.86%	3.991%
7	9.198	1170	1175	1178	rBV	2399320	2000232	81.59%	12.591%
8	9.875	1286	1290	1294	rBV	819579	695697	28.38%	4.379%
9	10.663	1420	1424	1433	rBV	1574150	1340625	54.69%	8.439%
10	11.363	1539	1543	1546	rBV	975127	774696	31.60%	4.876%
11	11.892	1629	1633	1643	rBV	219633	235996	9.63%	1.485%
12	12.610	1751	1755	1763	rVB6	29731	57518	2.35%	0.362%
13	12.675	1763	1766	1774	rBV	84551	100697	4.11%	0.634%
14	12.845	1791	1795	1805	rBV	17886	39330	1.60%	0.248%
15	12.951	1809	1813	1817	rBV	2790796	2451534	100.00%	15.431%
16	13.857	1965	1967	1969	rBV	35690	40538	1.65%	0.255%
17	13.886	1969	1972	1981	rVB2	88060	174878	7.13%	1.101%
18	14.004	1988	1992	1996	rBV	815624	708767	28.91%	4.461%
19	14.104	2005	2009	2013	rBV	342984	324231	13.23%	2.041%
20	14.480	2071	2073	2076	rBV	65879	51254	2.09%	0.323%
21	15.133	2181	2184	2189	rVB	92379	108779	4.44%	0.685%
22	15.468	2237	2241	2246	rBV	400596	488228	19.92%	3.073%
23	15.951	2320	2323	2328	rVB	85779	120255	4.91%	0.757%
24	17.286	2547	2550	2558	rVB5	119556	243489	9.93%	1.533%

Sum of corrected areas: 15886666

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
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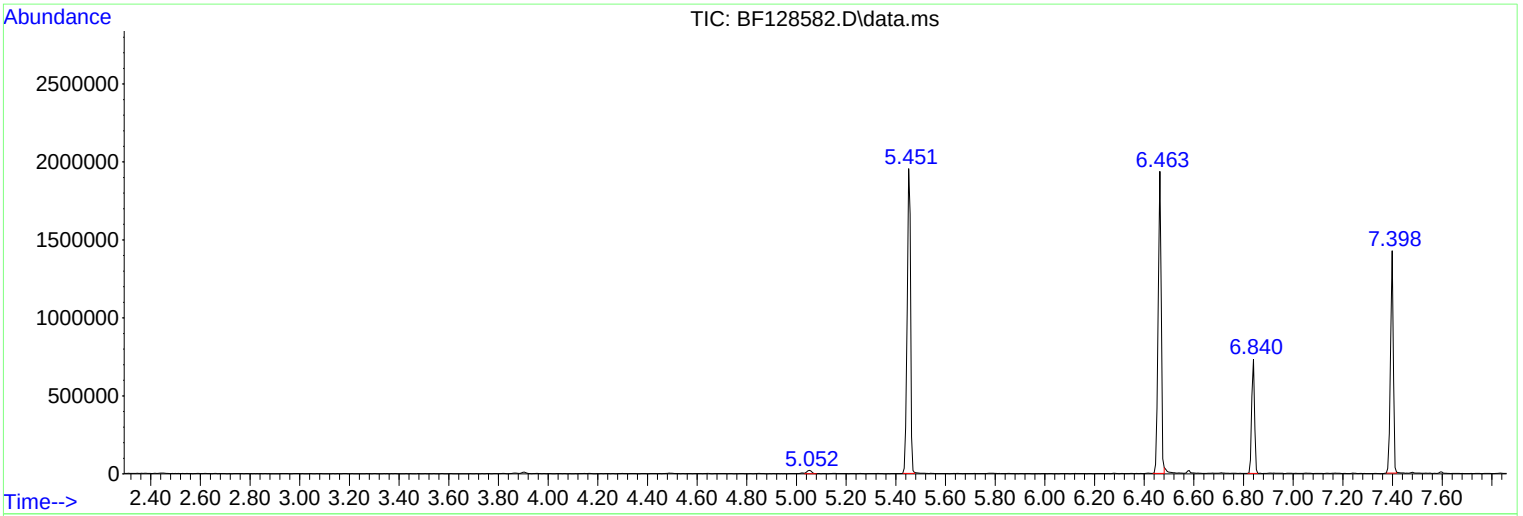
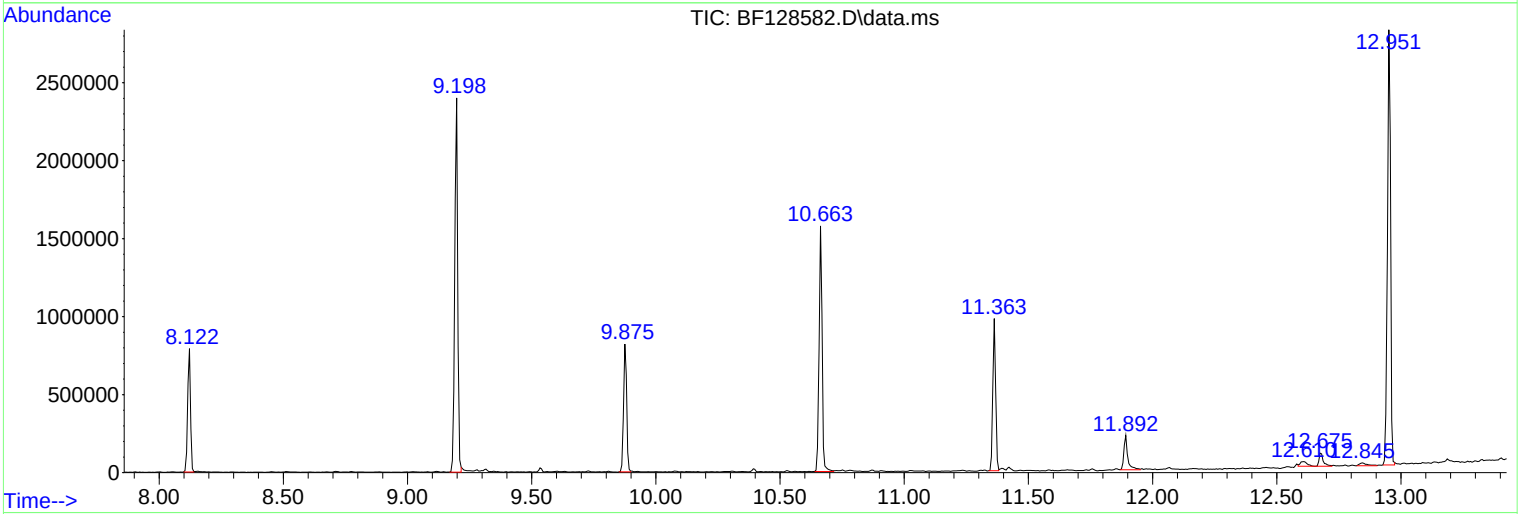
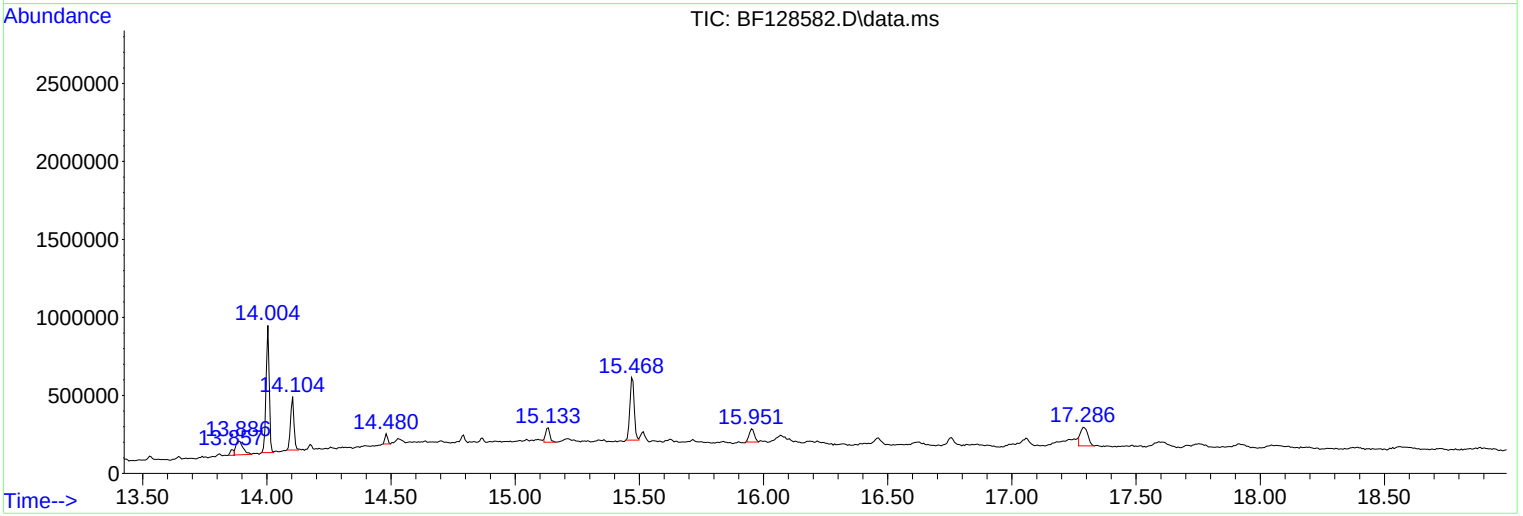
BNA_F
ClientSampleId :
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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Operator : CG\JU
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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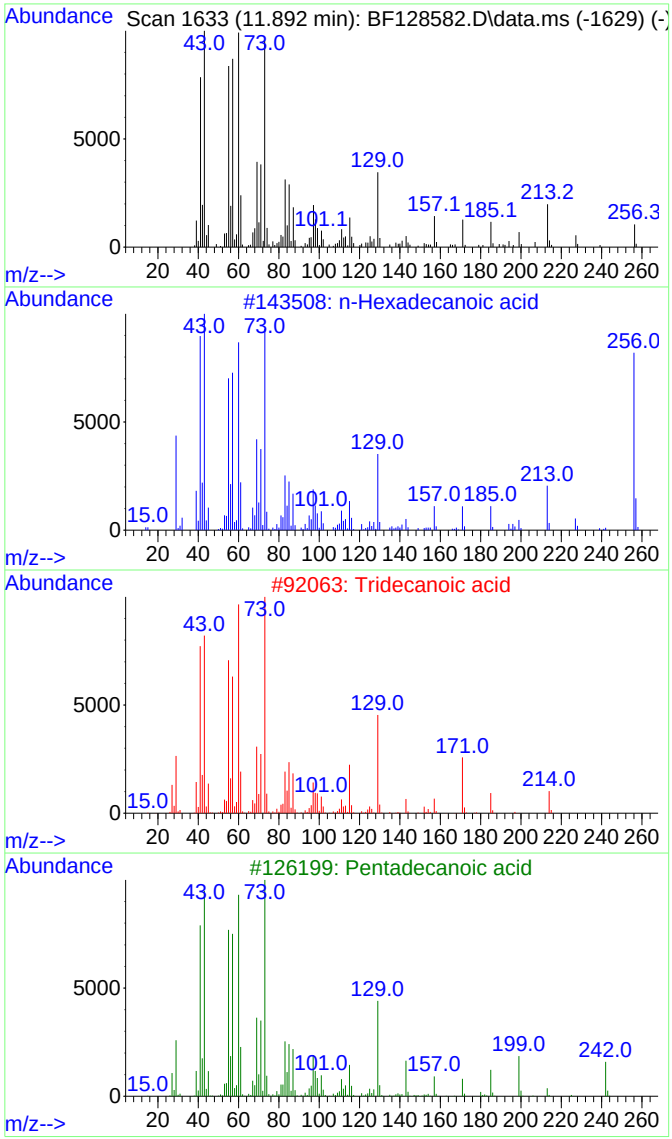
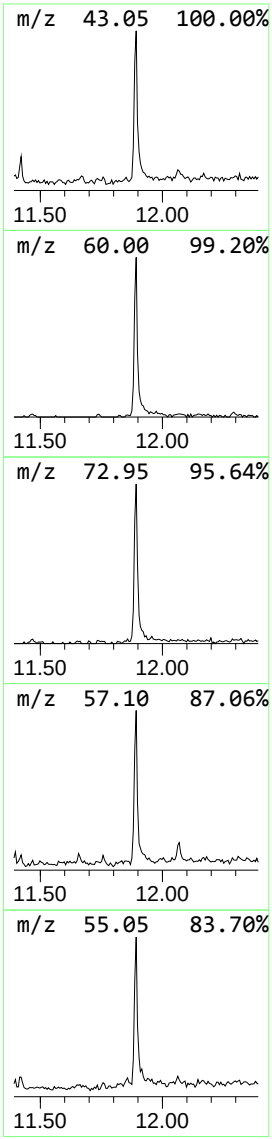
Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	6.09 ng	235996	Phenanthrene-d10	11.363

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Data File : BF128582.D
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Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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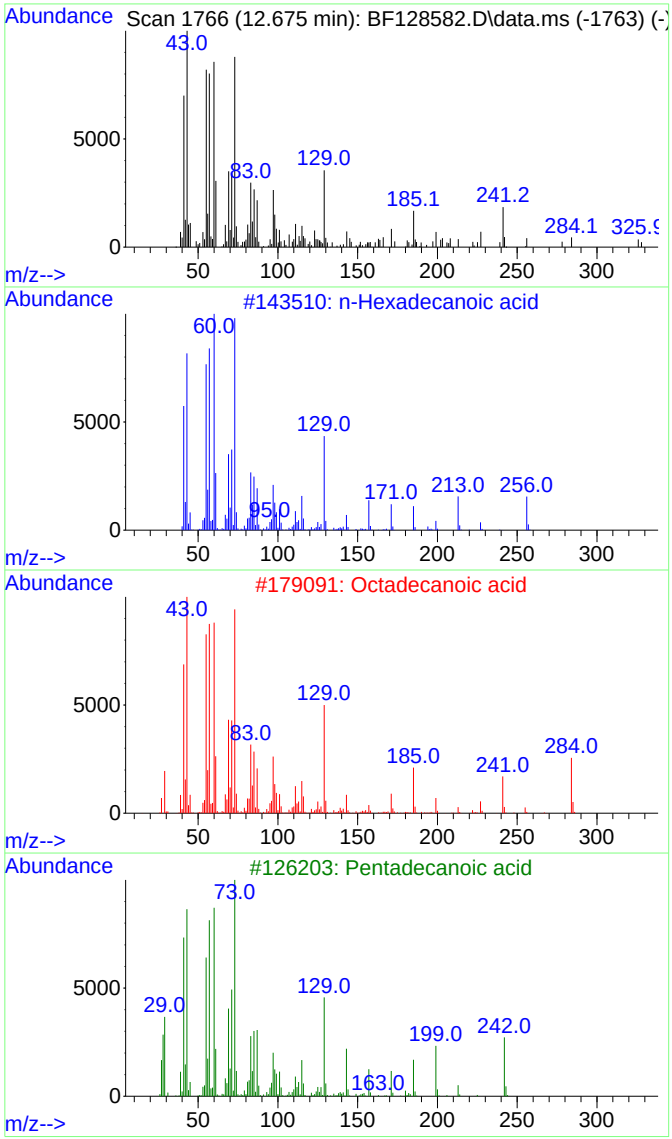
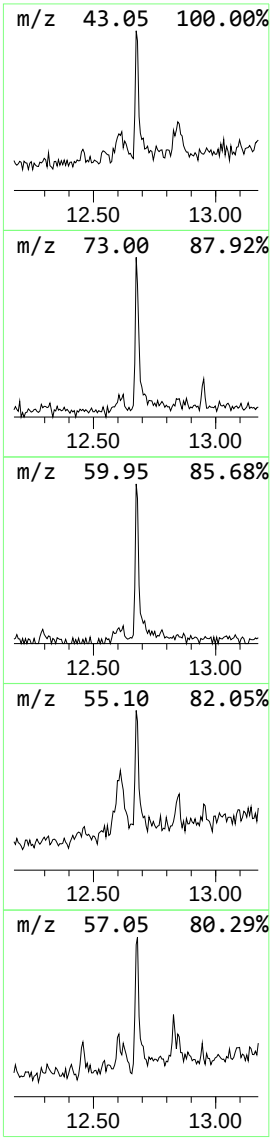
Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.675	2.60 ng	100697	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
5	Heneicosanoic acid	326	C21H42O2	002363-71-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128582.D
Acq On : 29 May 2022 20:30
Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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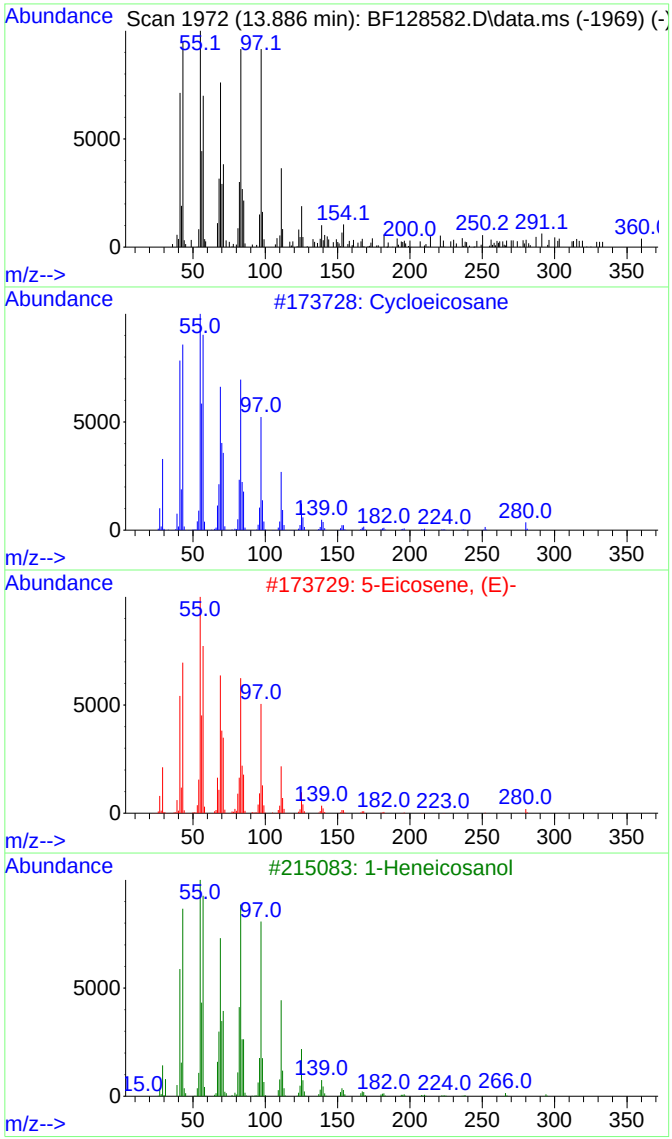
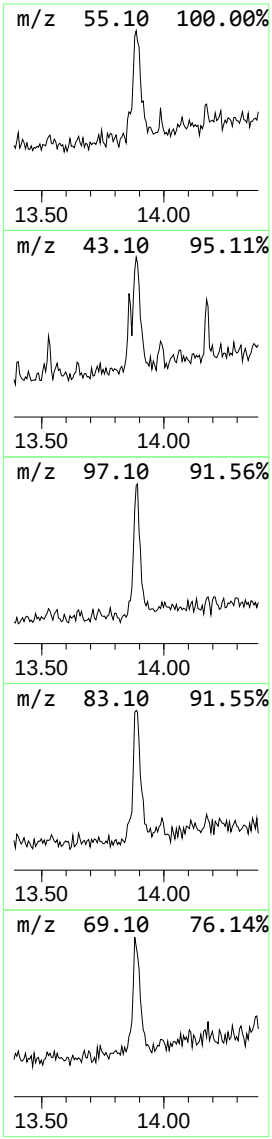
Peak Number 3 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.93 ng	174878	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	83
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	83
3	1-Heneicosanol	312	C21H44O	015594-90-8	83
4	1-Tricosene	322	C23H46	018835-32-0	83
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128582.D
Acq On : 29 May 2022 20:30
Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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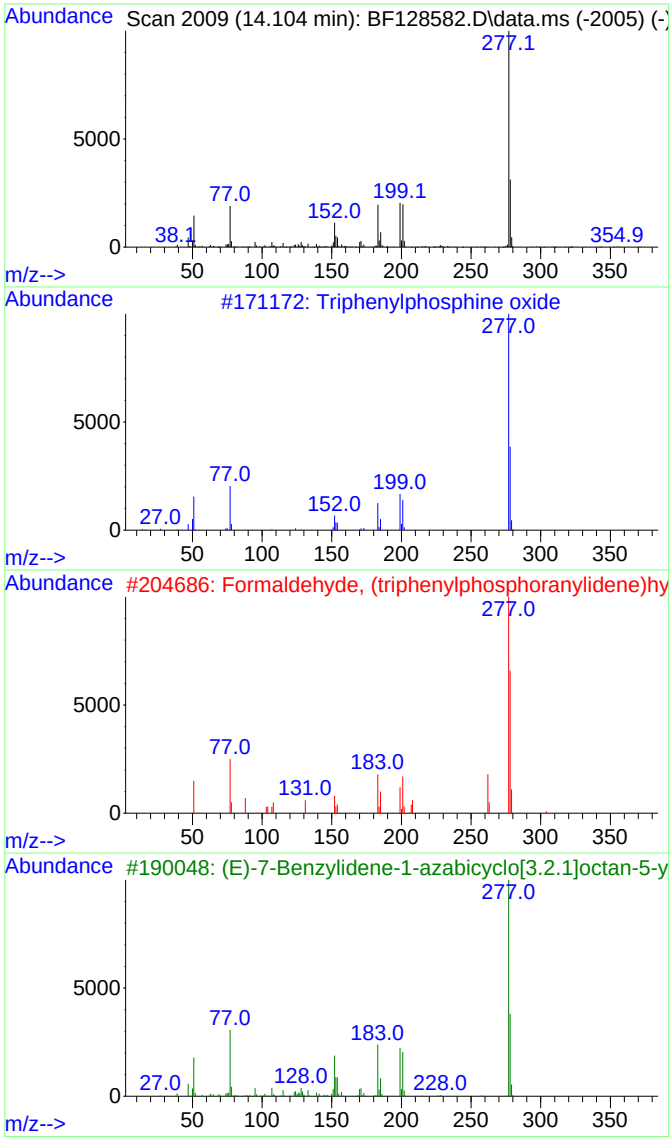
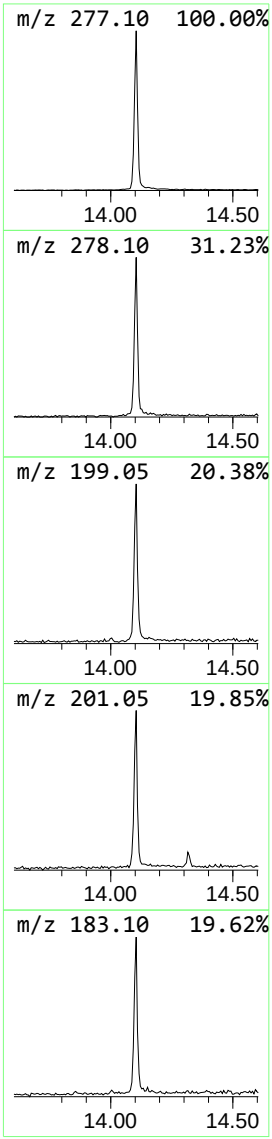
Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	9.15 ng	324231	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	53
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	52
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128582.D
Acq On : 29 May 2022 20:30
Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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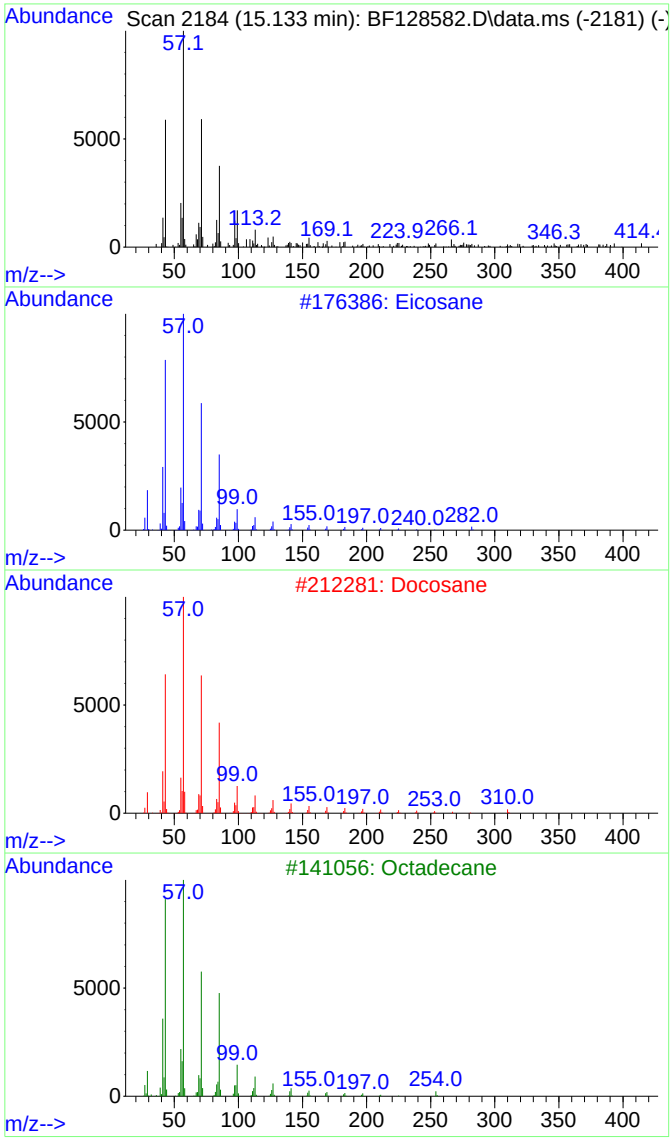
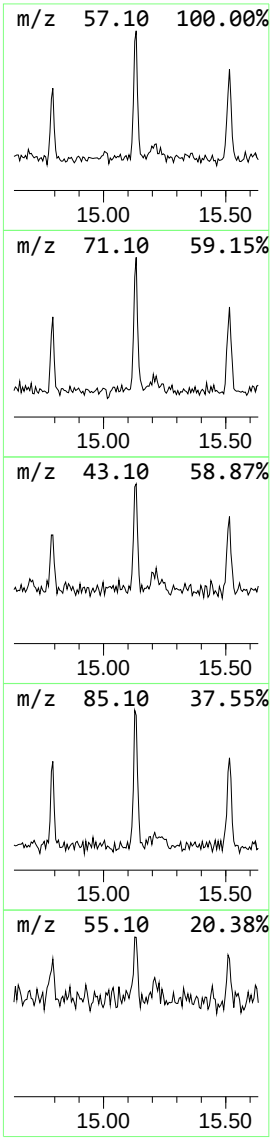
Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	4.46 ng	108779	Perylene-d12	15.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Docosane	310	C22H46	000629-97-0	93
3	Octadecane	254	C18H38	000593-45-3	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	Nonadecane	268	C19H40	000629-92-5	90





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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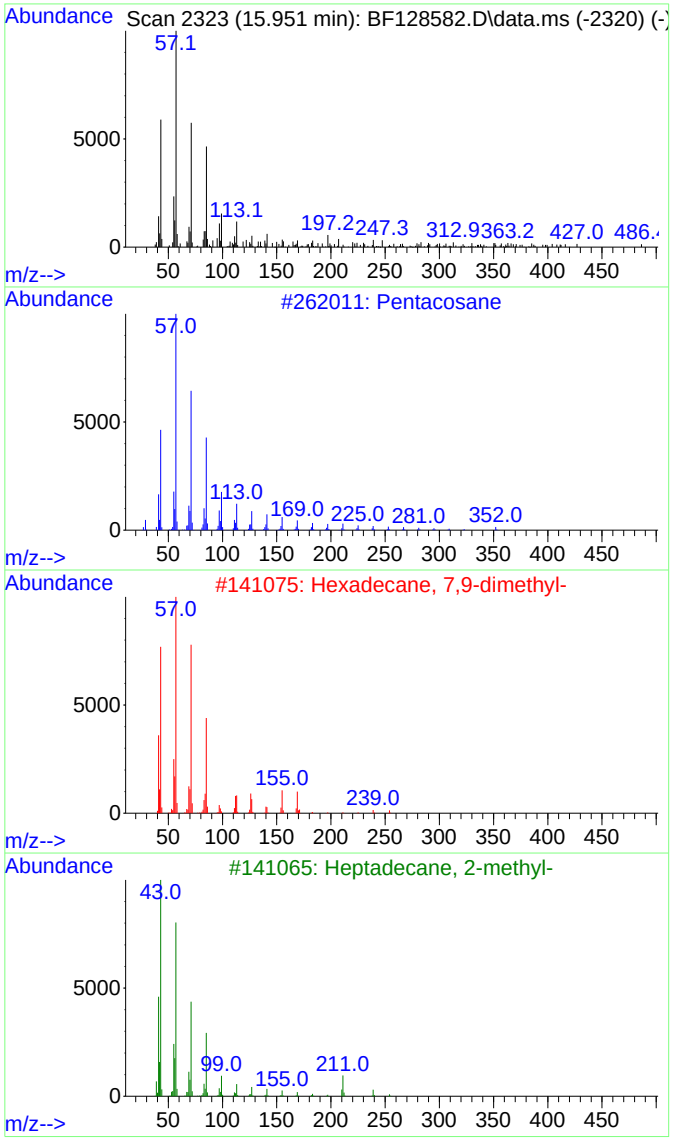
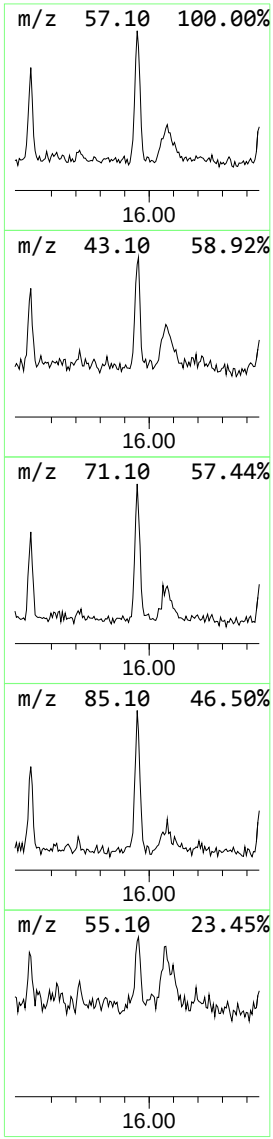
Peak Number 6 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	4.93 ng	120255	Perylene-d12	15.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	86
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	81
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	81
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	81
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	74





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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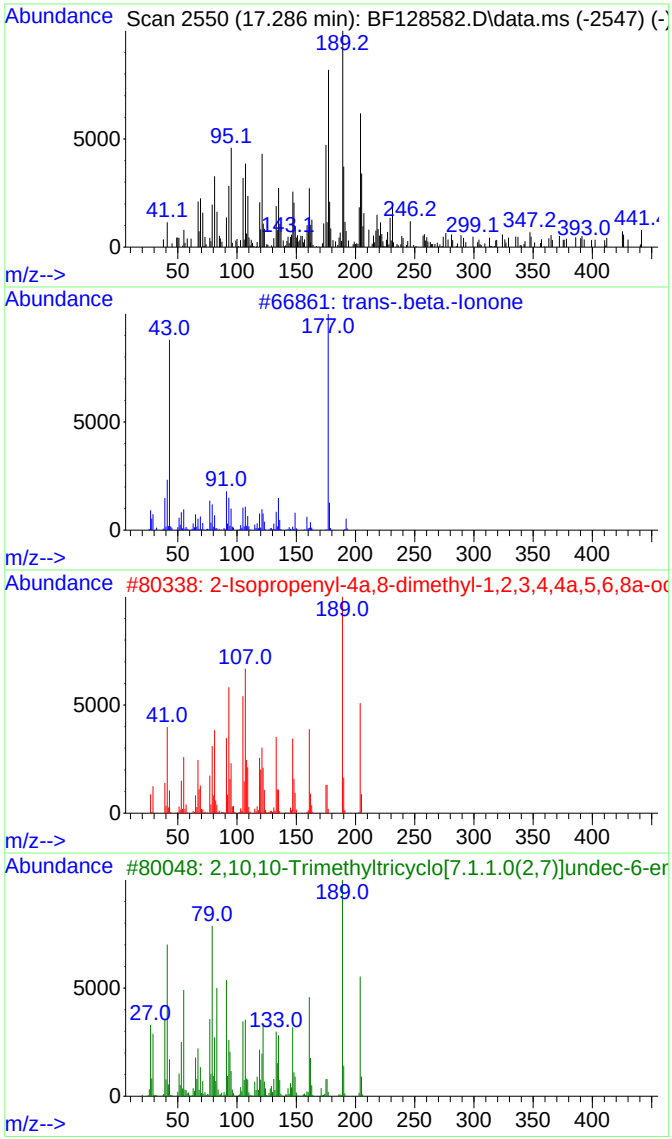
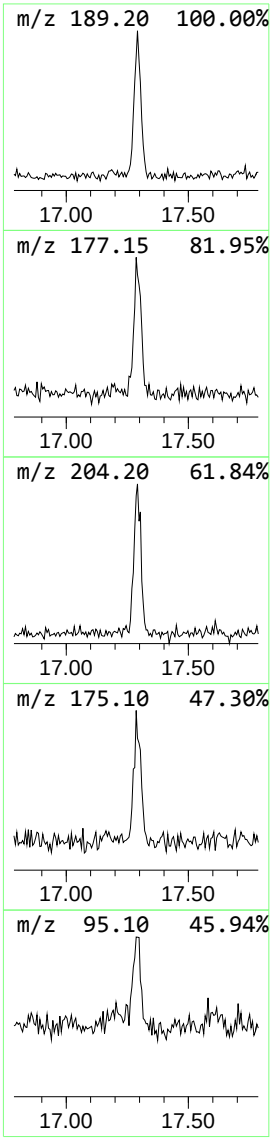
Peak Number 7 trans-.beta.-Ionone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	9.97 ng	243489	Perylene-d12	15.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-.beta.-Ionone	192	C13H20O	000079-77-6	83
2	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	50
3	2,10,10-Trimethyltricyclo[7.1.1....	204	C14H20O	1000210-81-9	38
4	2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	38
5	.beta.-Oplopenone	220	C15H24O	028305-60-4	30





Tentatively Identified Compound (LSC) summary

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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 ...	11.892	6.1	ng	235996	4	11.363	774696	20.0
Octadecanoic acid	12.675	2.6	ng	100697	4	11.363	774696	20.0
Cycloeicosane	13.886	4.9	ng	174878	5	14.004	708767	20.0
Triphenylphosph...	14.104	9.2	ng	324231	5	14.004	708767	20.0
Eicosane	15.133	4.5	ng	108779	6	15.469	488228	20.0
Pentacosane	15.951	4.9	ng	120255	6	15.469	488228	20.0
trans-.beta.-Io...	17.286	10.0	ng	243489	6	15.469	488228	20.0