LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134360.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	5	11	18	rVB	393900	495779	19.11%	2.907%
2	5.104	510	513	524	rBV	25680	36542	1.41%	0.214%
3	5.481	573	577	580	rBV	1984664	1951801	75.22%	11.445%
4	6.486	742	748	751	rBV	1964398	2034789	78.41%	11.931%
5	6.839	804	808	814	rBV	585754	484820	18.68%	2.843%
6	7.404	899	904	907	rBV	1503221	1327487	51.16%	7.784%
7	8.116	1021	1025	1028	rBV	791004	619822	23.89%	3.634%
8	9.198	1204	1209	1212	rBV	2810662	2594940	100.00%	15.216%
9	9.304	1224	1227	1232	rVB	30531	29293	1.13%	0.172%
10	9.874	1320	1324	1327	rBV	817905	643760	24.81%	3.775%
11	10.669	1455	1459	1463	rBV	1645169	1553429	59.86%	9.109%
12	11.368	1574	1578	1580	rBV	729496	586383	22.60%	3.438%
13	11.392	1580	1582	1586	rVB	180387	141728	5.46%	0.831%
14	11.898	1665	1668	1680	rVB2	315259	294538	11.35%	1.727%
15	12.204	1717	1720	1724	rBV	28552	29115	1.12%	0.171%
16	12.592	1782	1786	1792	rBV	166603	173464	6.68%	1.017%
17	12.686	1799	1802	1807	rBV	50558	57808	2.23%	0.339%
18	12.821	1819	1825	1829	rBV	138607	140115	5.40%	0.822%
19	12.968	1845	1850	1853	rBV	2395111	2080832	80.19%	12.201%
20	13.892	2001	2007	2022	rBV5	78601	194629	7.50%	1.141%
21	14.004	2022	2026	2027	rBV2	27857	28399	1.09%	0.167%
22	14.033	2027	2031	2034	rVV	494150	494518	19.06%	2.900%
23	14.057	2034	2035	2041	rVB	63579	43678	1.68%	0.256%
24	14.121	2042	2046	2051	rBV	64864	64913	2.50%	0.381%
25	14.186	2054	2057	2063	rBV	29525	36283	1.40%	0.213%
26	14.498	2107	2110	2114	rBV2	35953	35167	1.36%	0.206%
27	14.545	2114	2118	2121	rBV5	29012	41357	1.59%	0.243%
28	15.092	2207	2211	2214	rBV2	45724	63483	2.45%	0.372%
29	15.156	2219	2222	2227	rVB	52671	70450	2.71%	0.413%
30	15.409	2261	2265	2272	rVB	26689	38008	1.46%	0.223%
31	15.474	2272	2276	2281	rVB	33296	47815	1.84%	0.280%
32	15.539	2282	2287	2295	rBV	277196	375933	14.49%	2.204%
33	15.768	2323	2326	2331	rVB5	27605	41493	1.60%	0.243%
34	16.015	2364	2368	2376	rVB3	46047	76717	2.96%	0.450%
35	16.145	2384	2390	2401	rBV3	21713	66098	2.55%	0.388%
36	16.856	2505	2511	2521	rBV9	23826	58608	2.26%	0.344%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

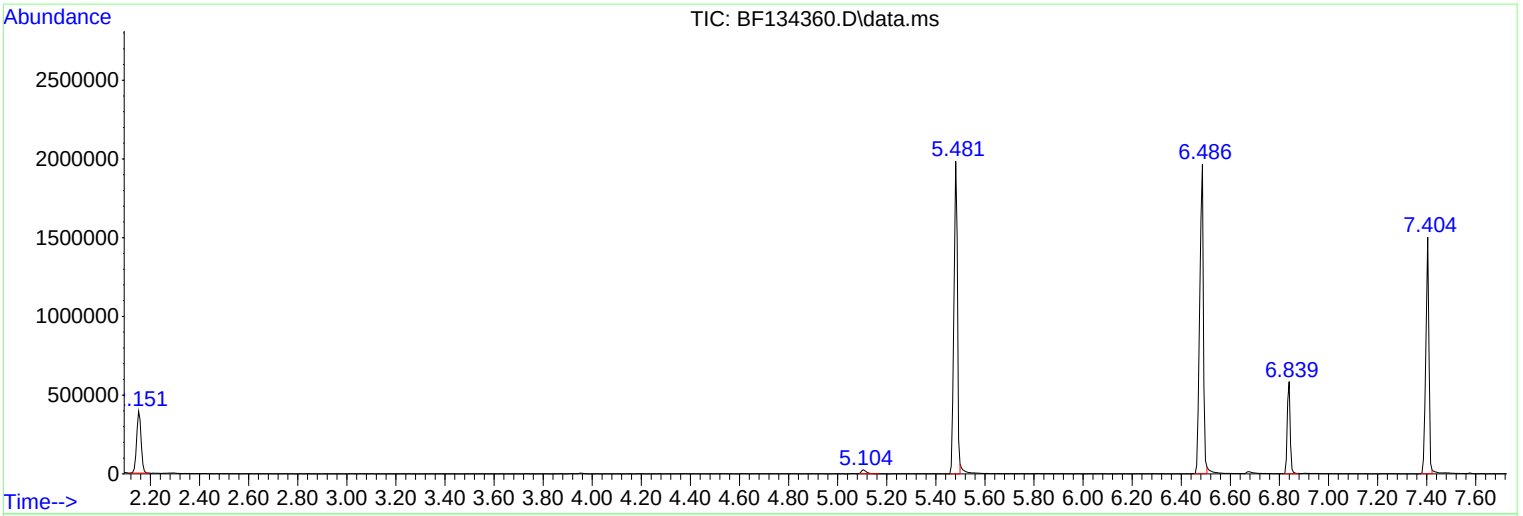
Sum of corrected areas: 17053994

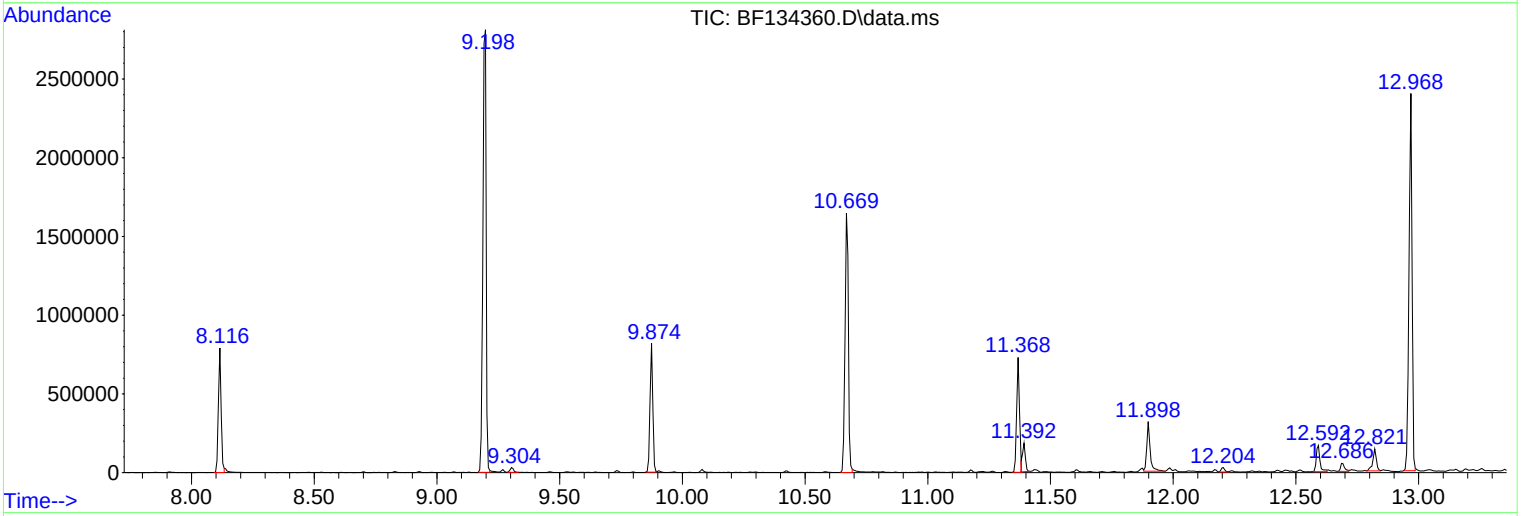
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

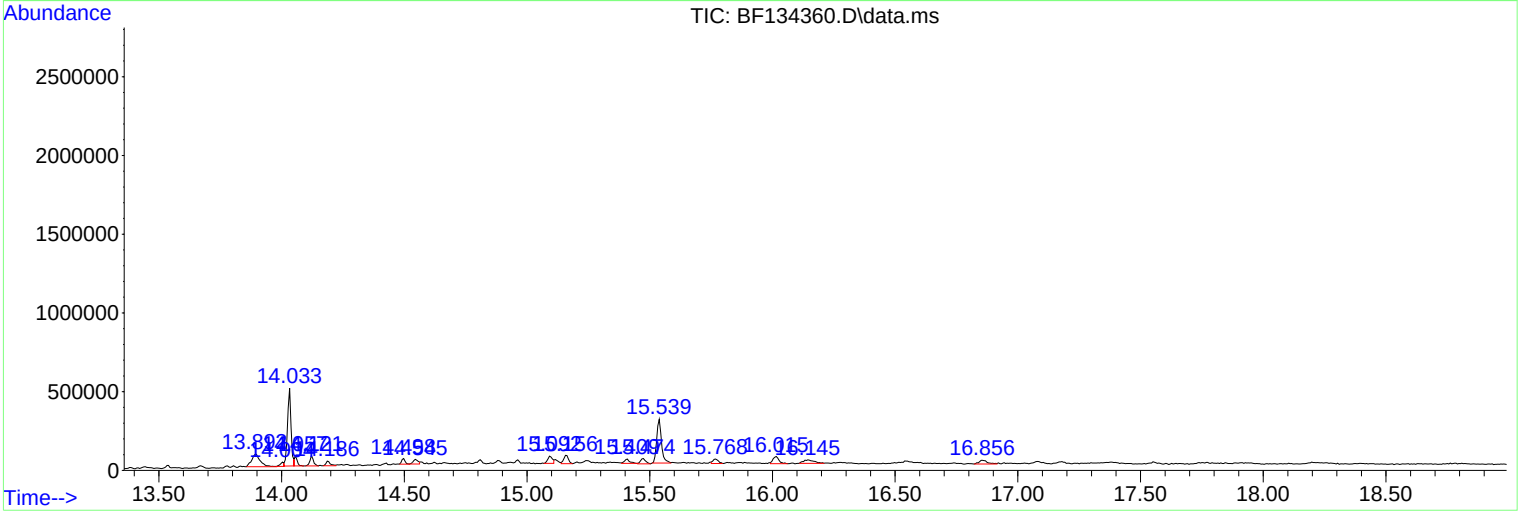
Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

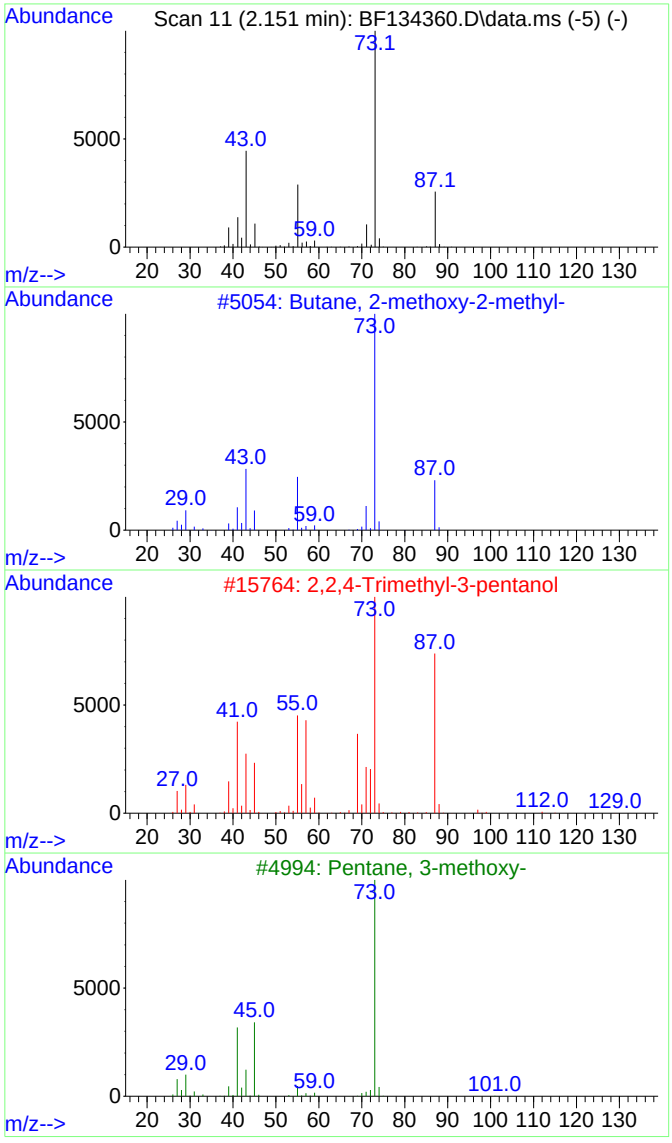
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

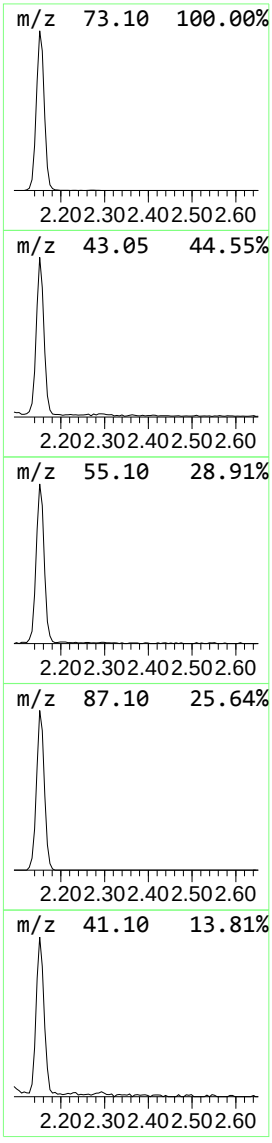
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	20.45 ng	495779	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

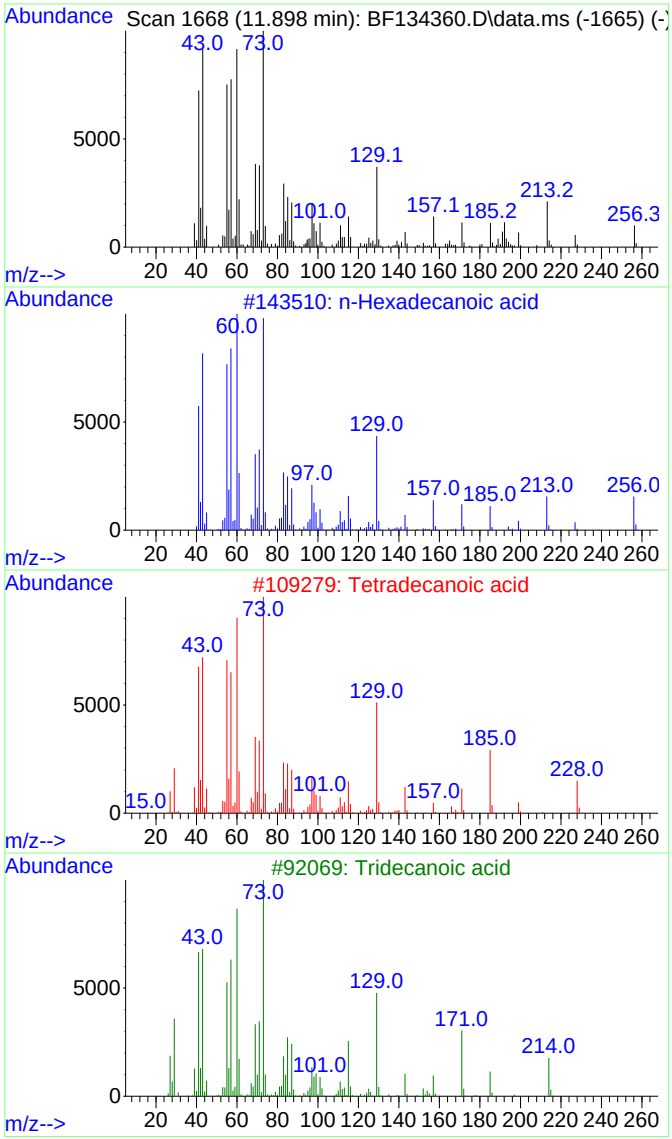
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

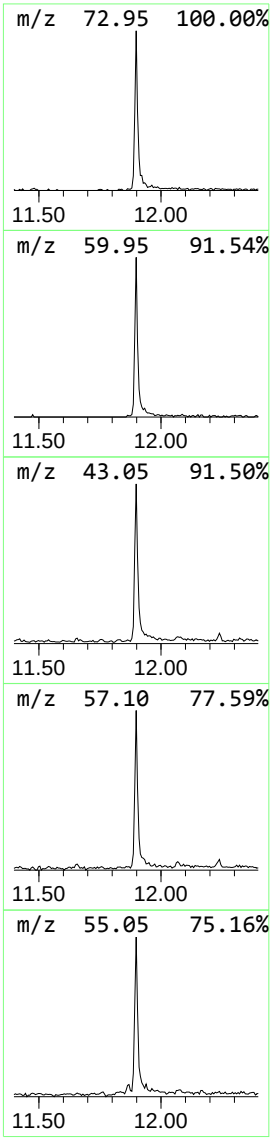
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	10.05 ng	294538	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

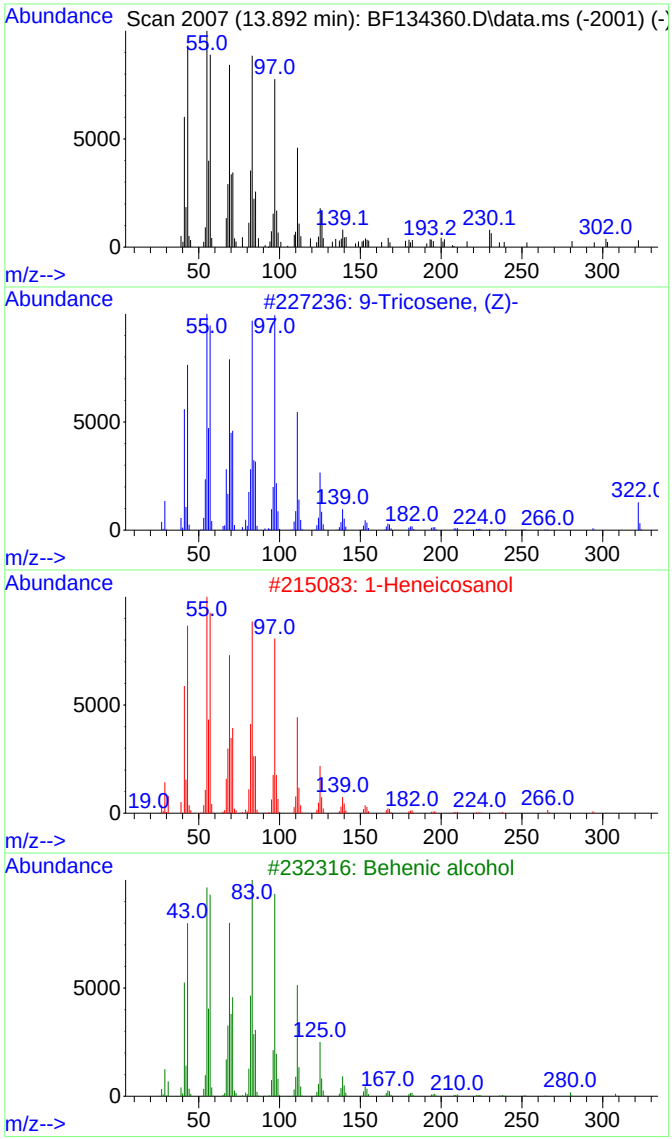
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

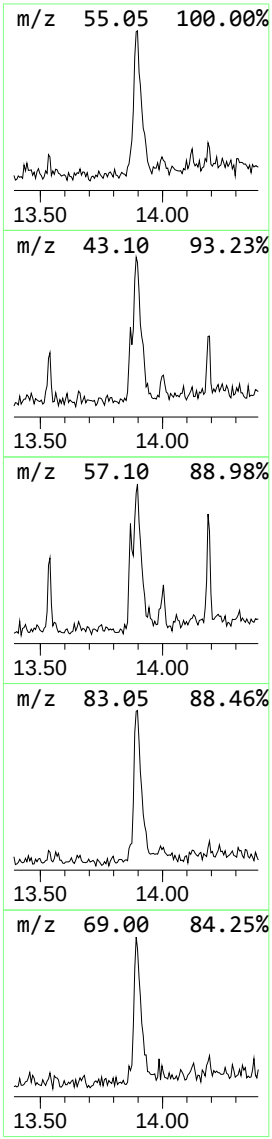
****

Peak Number 3 9-Tricosene, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	7.87 ng	194629	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	1-Tricosene	322	C23H46	018835-32-0	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

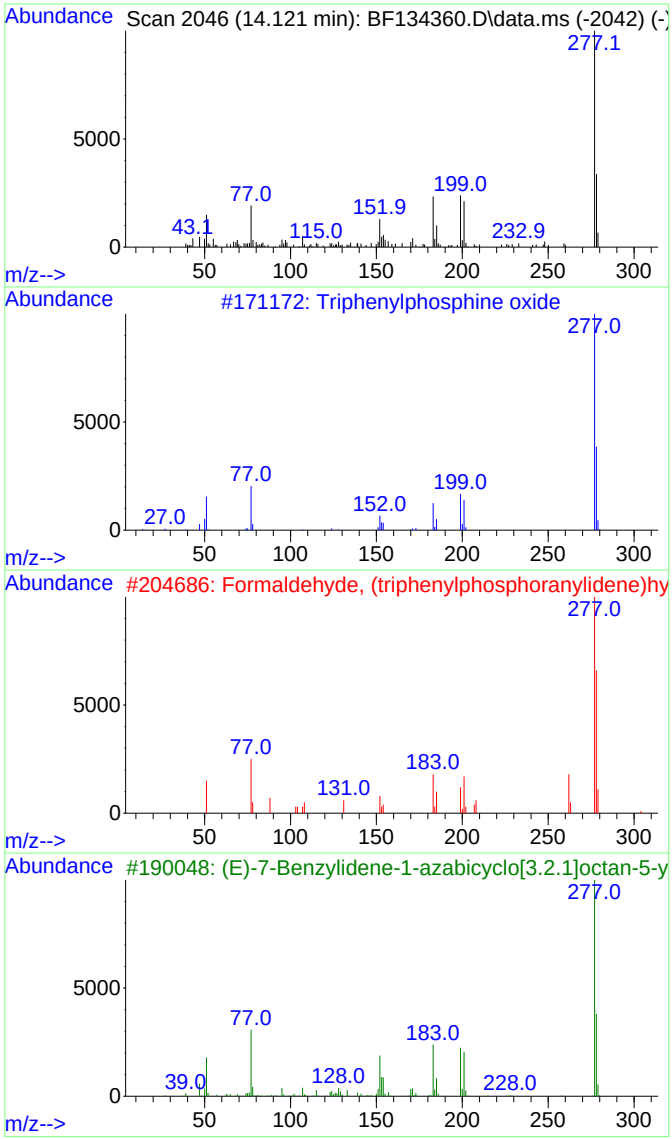
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

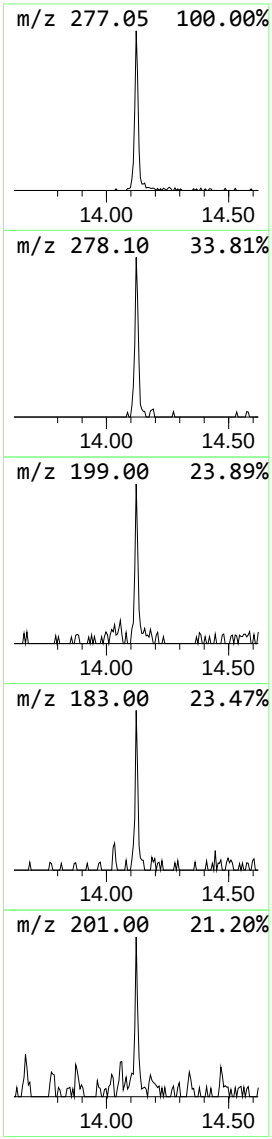
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Triphenylphosphine oxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	2.63 ng	64913	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	47
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
5	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

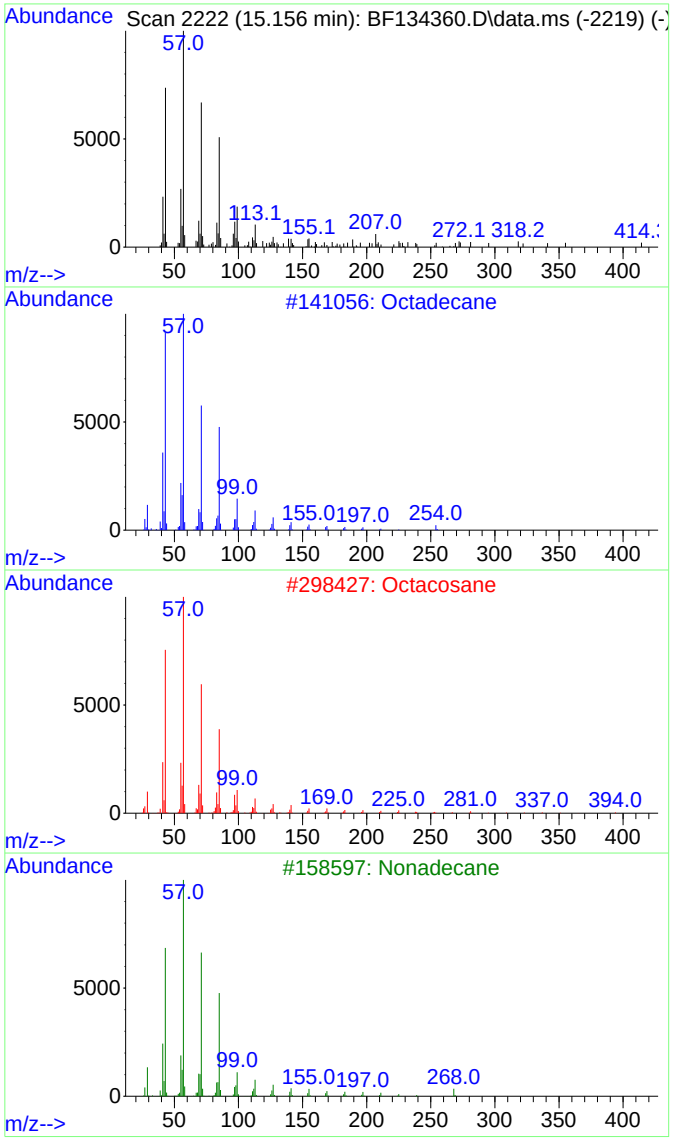
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

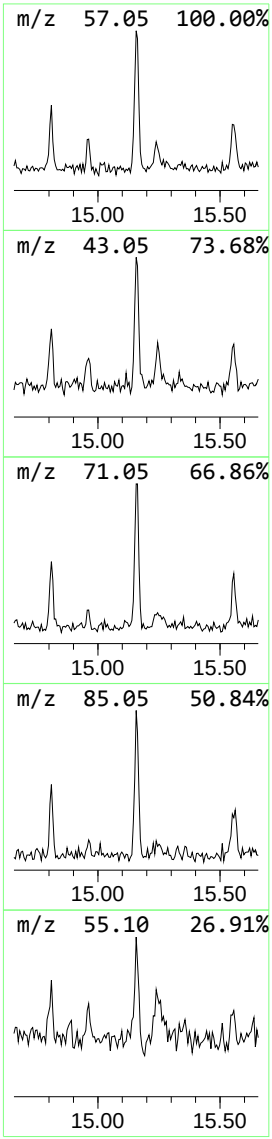
****

Peak Number 5 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.156	3.75 ng	70450	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Octacosane	394	C28H58	000630-02-4	86
3	Nonadecane	268	C19H40	000629-92-5	86
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





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Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

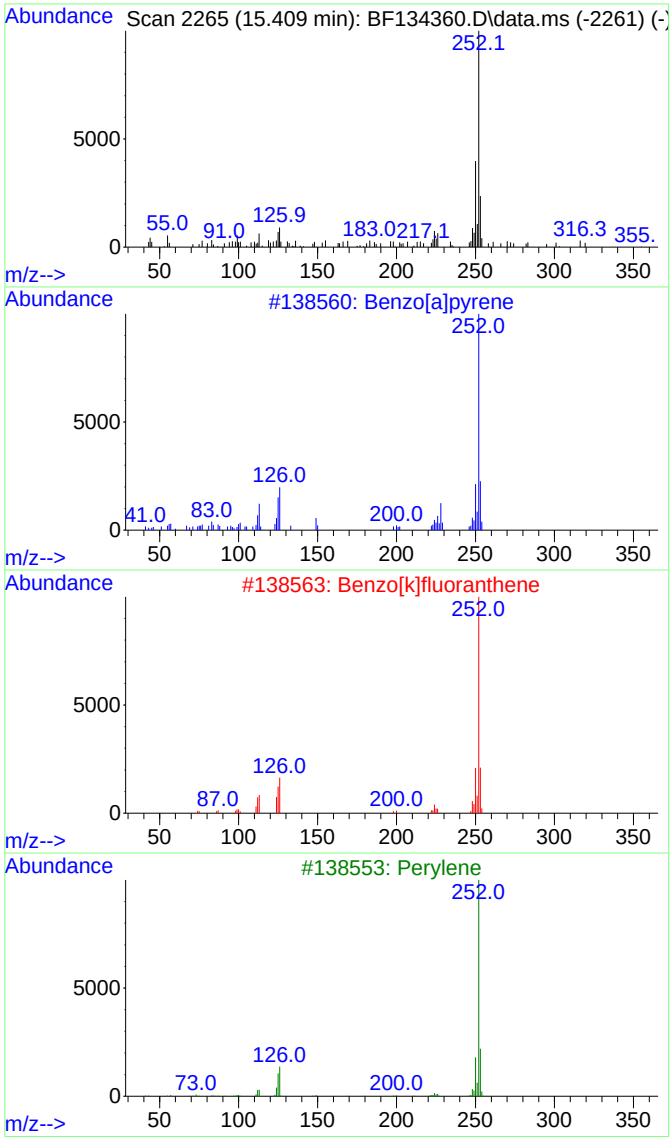
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

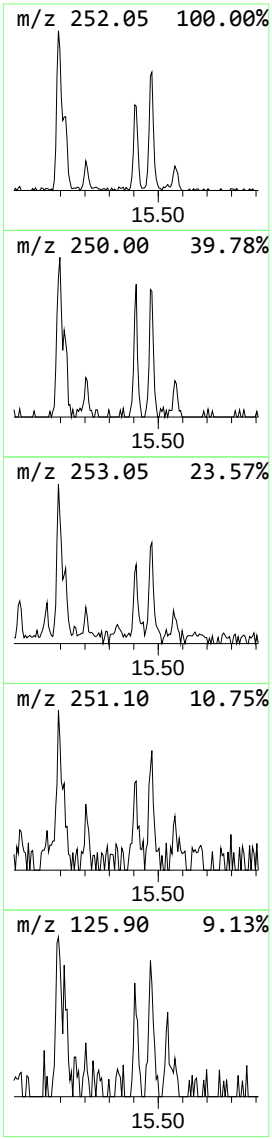
****

Peak Number 6 (1-Cyclopentenyl)ferrocene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.409	2.02 ng	38008	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	70
3	Perylene	252	C20H12	000198-55-0	70
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	64
5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	59





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Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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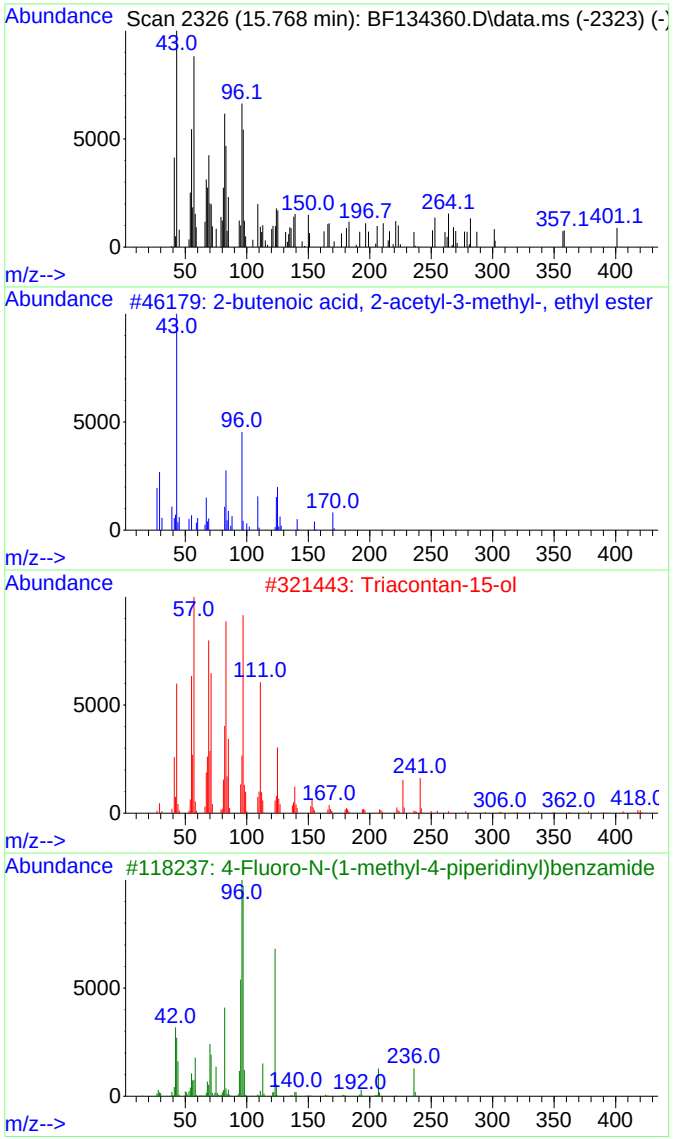
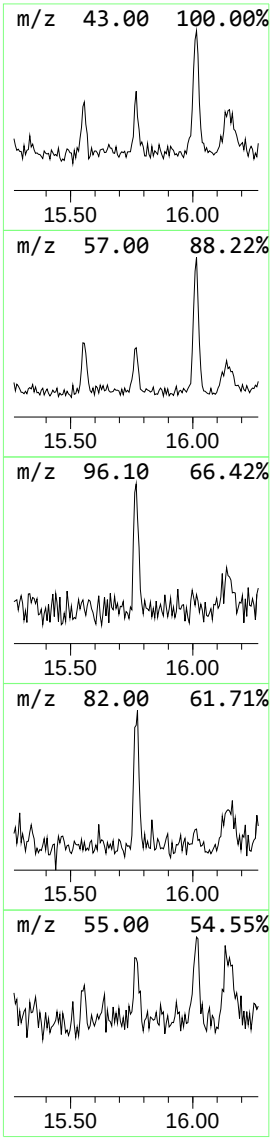
Peak Number 7 unknown15.768 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	2.21 ng	41493	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-butenoic acid, 2-acetyl-3-meth...	170	C9H14O3	1000404-58-0	43
2	Triacontan-15-ol	438	C30H62O	031849-26-0	38
3	4-Fluoro-N-(1-methyl-4-piperidin...	236	C13H17FN2O	210643-93-9	30
4	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	27
5	1-Decene, 10-bromo-	218	C10H19Br	062871-09-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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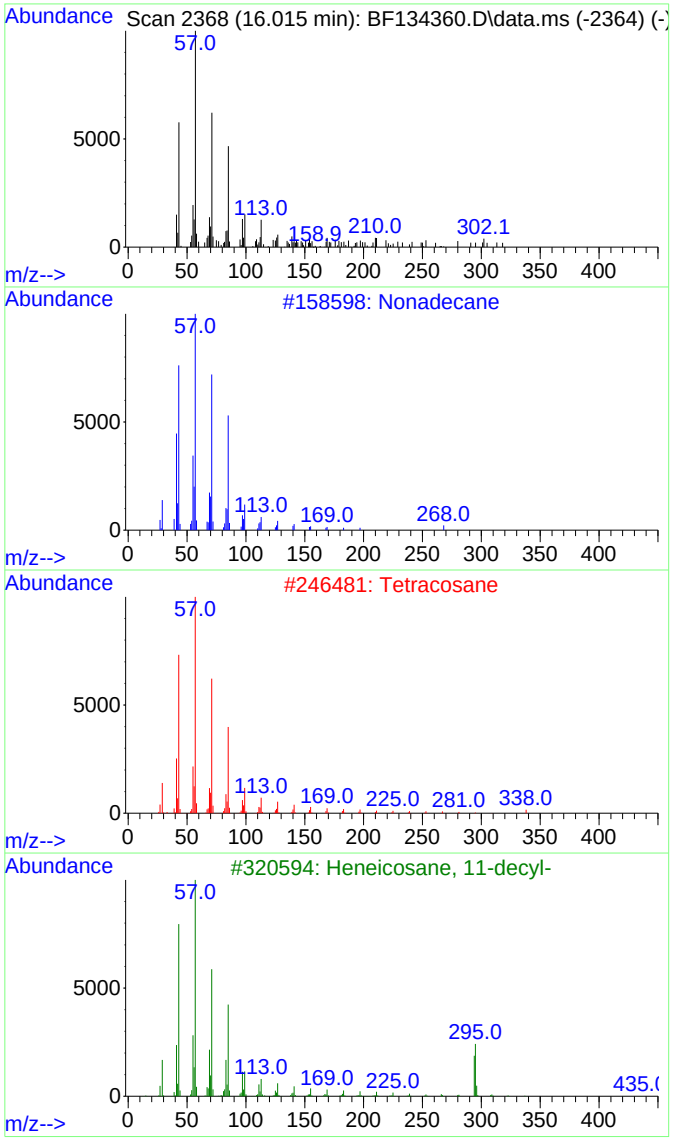
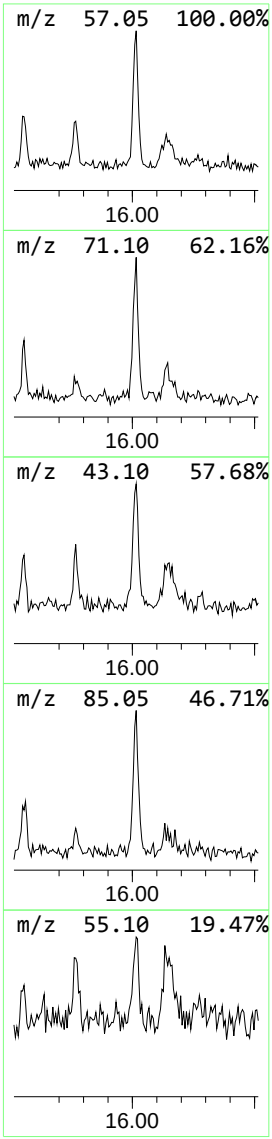
Peak Number 8 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	4.08 ng	76717	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Tetracosane	338	C24H50	000646-31-1	87
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Hexacosane	366	C26H54	000630-01-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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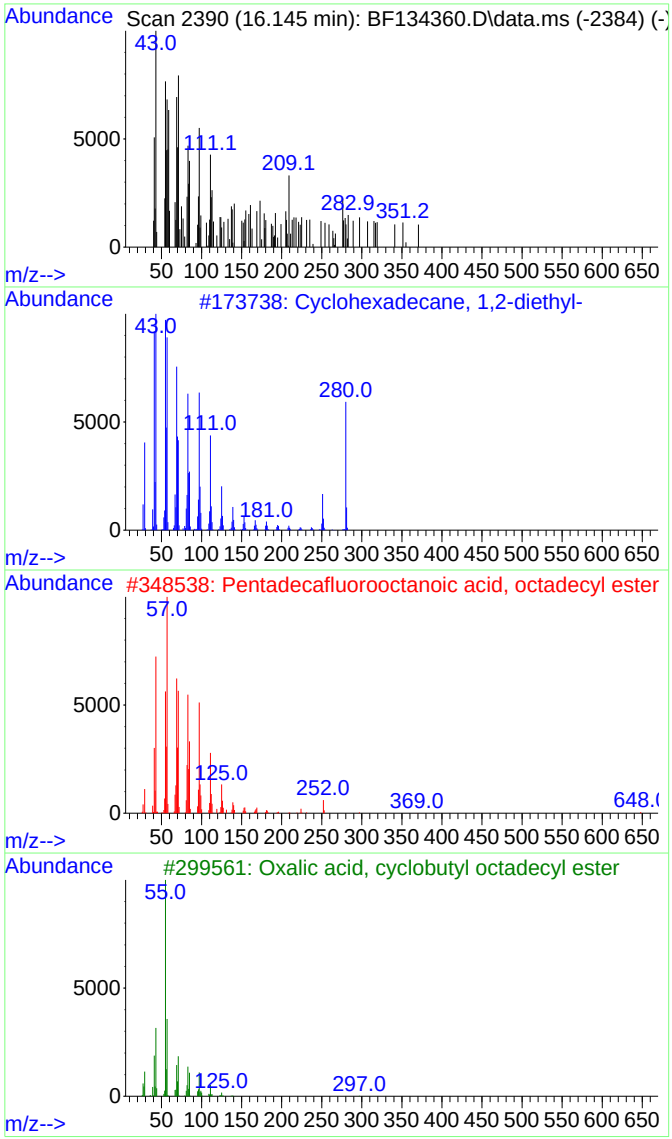
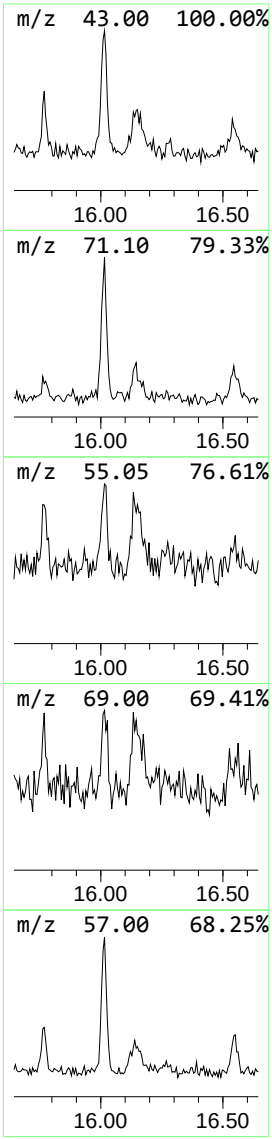
Peak Number 9 Cyclohexadecane, 1,2-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	3.52 ng	66098	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	59
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	52
3	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	46
4	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	38
5	1-Eicosene	280	C20H40	003452-07-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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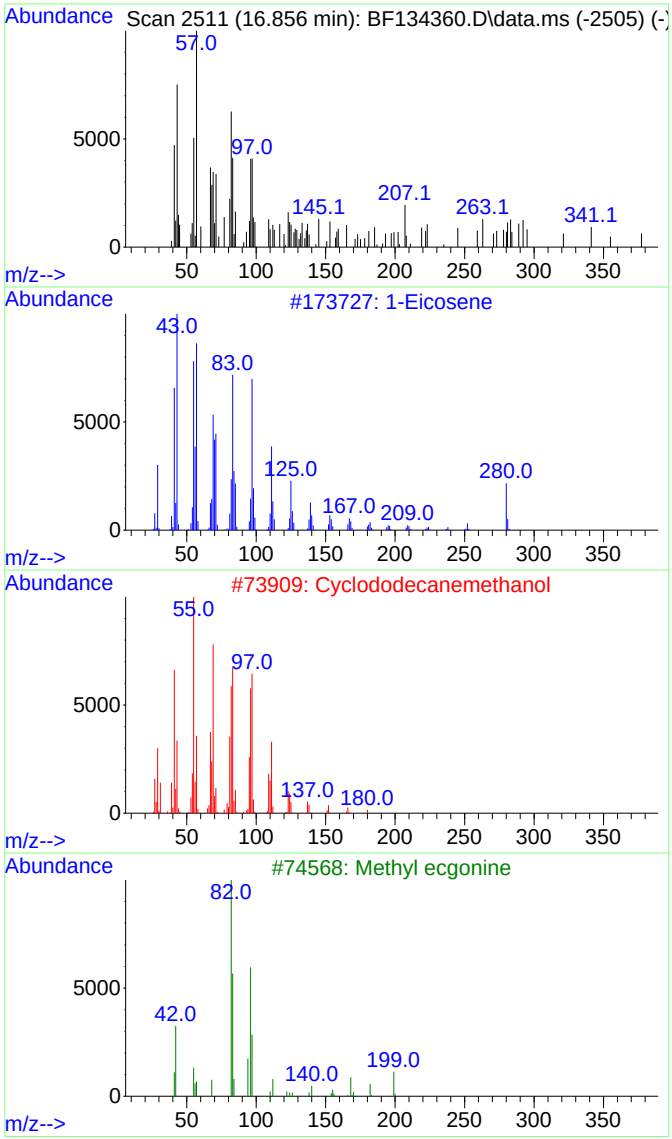
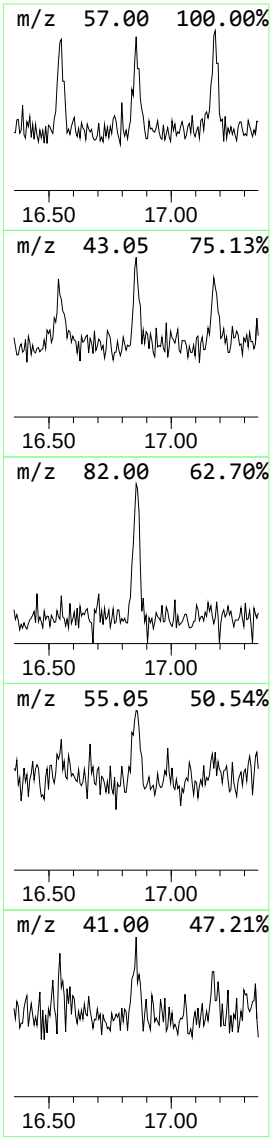
Peak Number 10 unknown16.856 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.856	3.12 ng	58608	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	41
2	Cyclododecanemethanol	198	C13H26O	001892-12-2	38
3	Methyl ecgonine	199	C10H17NO3	007143-09-1	38
4	Octadecanal	268	C18H36O	000638-66-4	38
5	1-Hexacosene	364	C26H52	018835-33-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134360.D
Acq On : 19 Jul 2023 15:50
Operator : CG\JU
Sample : 03597-20
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-51-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.151	20.4	ng	495779	1	6.839	484820	20.0
n-Hexadecanoic ...	11.898	10.1	ng	294538	4	11.368	586383	20.0
9-Tricosene, (Z)-	13.892	7.9	ng	194629	5	14.033	494518	20.0
Triphenylphosph...	14.121	2.6	ng	64913	5	14.033	494518	20.0
Octadecane	15.156	3.8	ng	70450	6	15.539	375933	20.0
(1-Cyclopenteny...	15.409	2.0	ng	38008	6	15.539	375933	20.0
unknown15.768	15.768	2.2	ng	41493	6	15.539	375933	20.0
Nonadecane	16.015	4.1	ng	76717	6	15.539	375933	20.0
Cyclohexadecane...	16.145	3.5	ng	66098	6	15.539	375933	20.0
unknown16.856	16.856	3.1	ng	58608	6	15.539	375933	20.0