LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031225\
Data File : BF141937.D
Acq On : 12 Mar 2025 14:26
Operator : RC/JU
Sample : Q1522-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141937.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	14	24	rVB	3102120	5008728	81.26%	11.359%
2	5.093	502	510	522	rVB2	43302	77273	1.25%	0.175%
3	5.492	567	578	592	rBV	1361861	1805987	29.30%	4.096%
4	5.828	625	635	652	rVB	142815	201038	3.26%	0.456%
5	6.128	681	686	693	rBV	162363	203772	3.31%	0.462%
6	6.492	742	748	757	rBV	840292	1081609	17.55%	2.453%
7	6.881	808	814	819	rBV	730003	936009	15.18%	2.123%
8	7.439	899	909	914	rBV	2170551	3037063	49.27%	6.887%
9	7.628	936	941	948	rBV2	40900	64731	1.05%	0.147%
10	7.757	957	963	978	rBV2	247980	440267	7.14%	0.998%
11	8.157	1026	1031	1047	rVB	979953	1293772	20.99%	2.934%
12	8.928	1157	1162	1175	rVB2	42330	87764	1.42%	0.199%
13	9.233	1208	1214	1219	rBV	4750685	6164082	100.00%	13.979%
14	9.492	1253	1258	1269	rVB	251186	314453	5.10%	0.713%
15	9.716	1292	1296	1314	rVB	56904	116431	1.89%	0.264%
16	9.910	1325	1329	1339	rVB	1137198	1473553	23.91%	3.342%
17	10.004	1339	1345	1356	rBV	34641	69174	1.12%	0.157%
18	10.627	1446	1451	1457	rVB	97602	125580	2.04%	0.285%
19	10.704	1457	1464	1469	rBV	2873106	3906490	63.38%	8.859%
20	11.398	1577	1582	1587	rVB	1177234	1464631	23.76%	3.321%
21	11.792	1643	1649	1654	rBV	999893	1263912	20.50%	2.866%
22	11.921	1664	1671	1691	rBV	691411	1116338	18.11%	2.532%
23	12.498	1760	1769	1777	rBV2	1041683	1734368	28.14%	3.933%
24	12.580	1778	1783	1786	rBV	467782	595511	9.66%	1.350%
25	12.639	1786	1793	1800	rVV	1484599	2670994	43.33%	6.057%
26	12.710	1800	1805	1818	rVB	336306	608985	9.88%	1.381%
27	12.986	1846	1852	1857	rBV	4584742	5985944	97.11%	13.575%
28	13.886	2000	2005	2013	rBV3	50085	119340	1.94%	0.271%
29	14.033	2025	2030	2039	rVB	750098	975226	15.82%	2.212%
30	15.509	2274	2281	2292	rBV	579393	941191	15.27%	2.134%
31	17.192	2561	2567	2579	rBV7	60100	211697	3.43%	0.480%

Sum of corrected areas: 44095913

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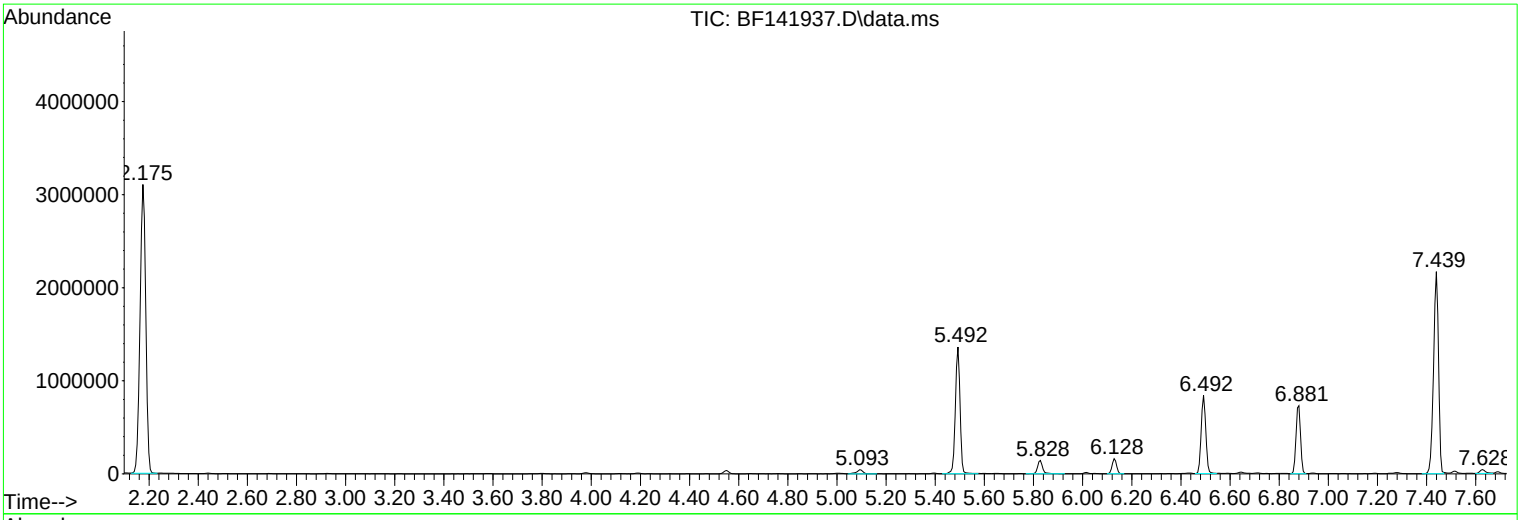
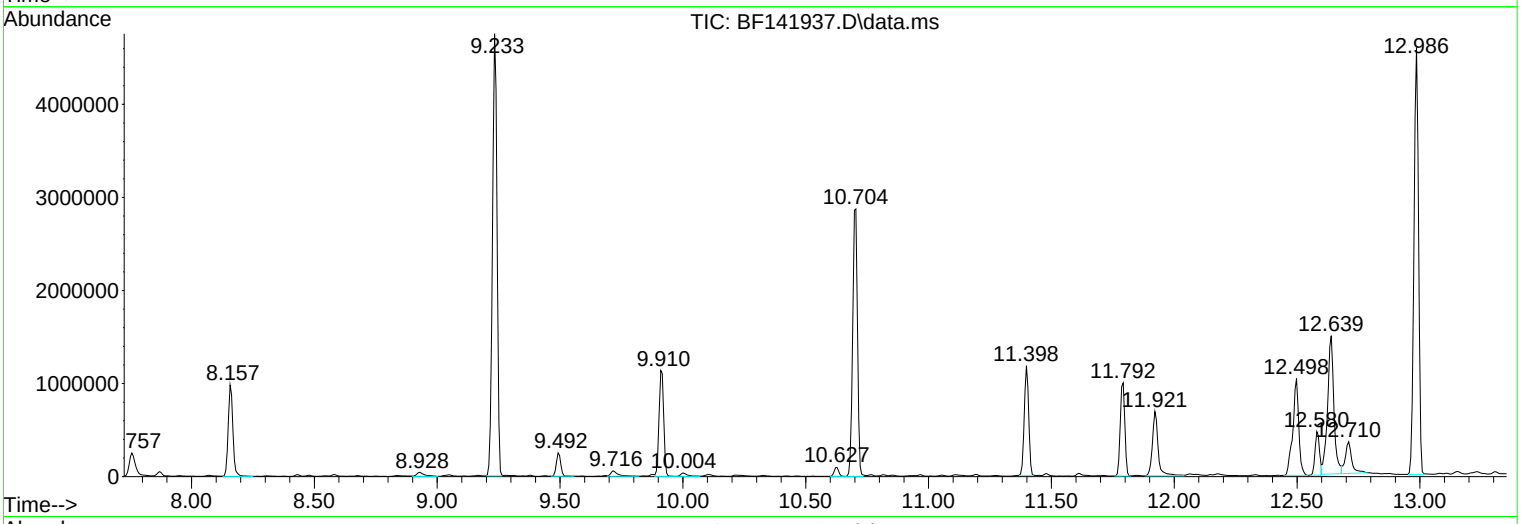
Misc :
ALS Vial : 8 Sample Multiplier: 1

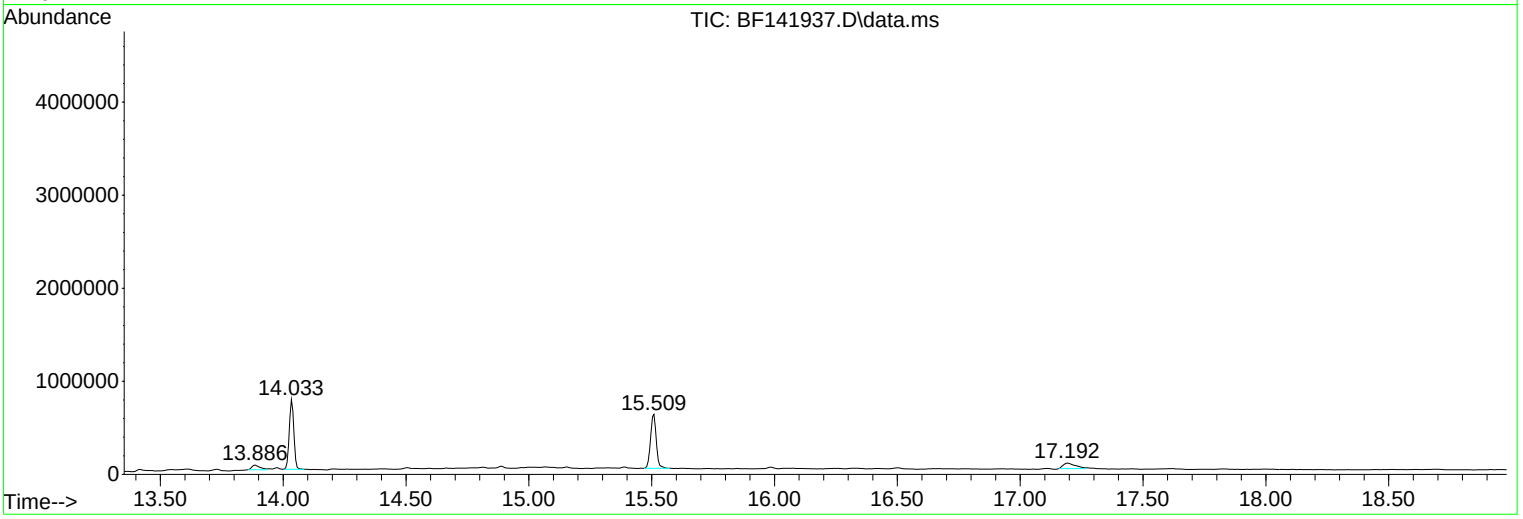
Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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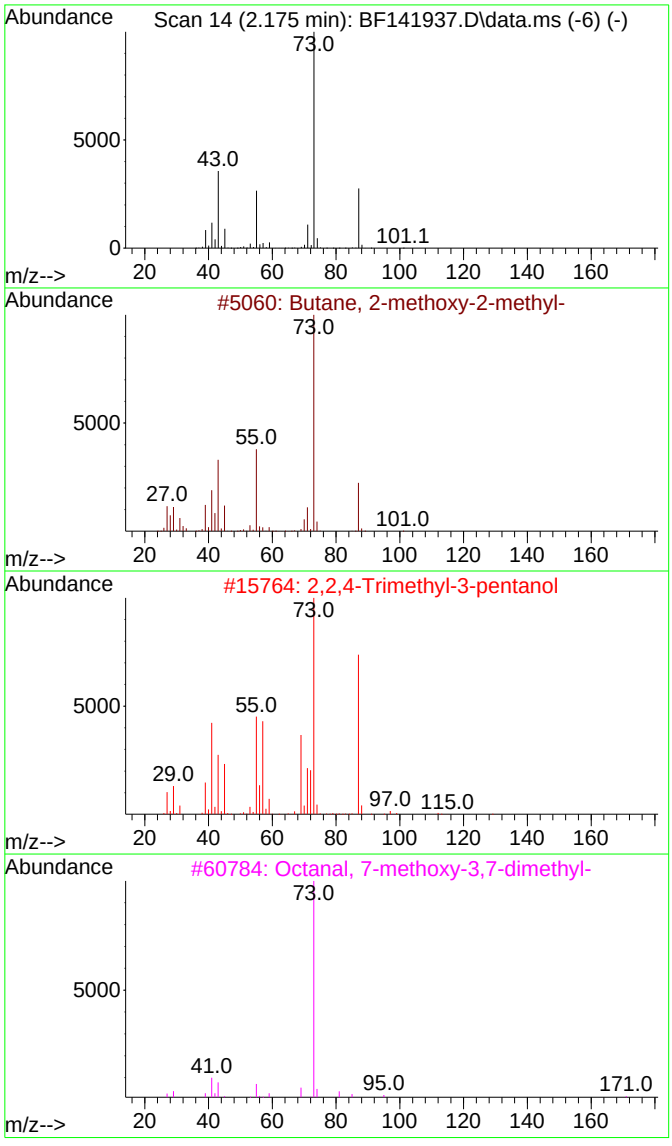
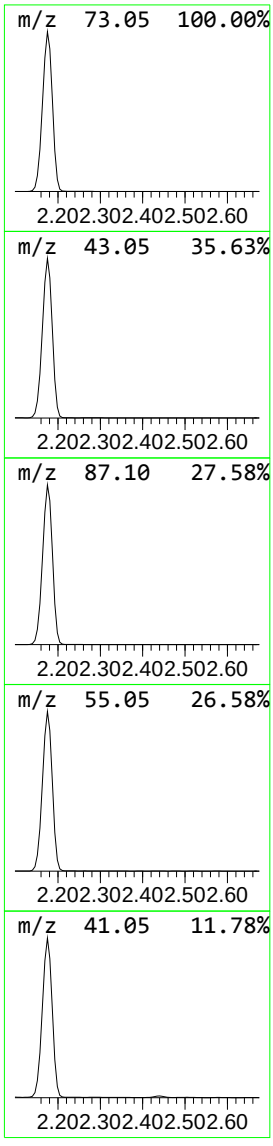
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	107.02 ng	5008730	1,4-Dichlorobenzene-d4	6.881

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	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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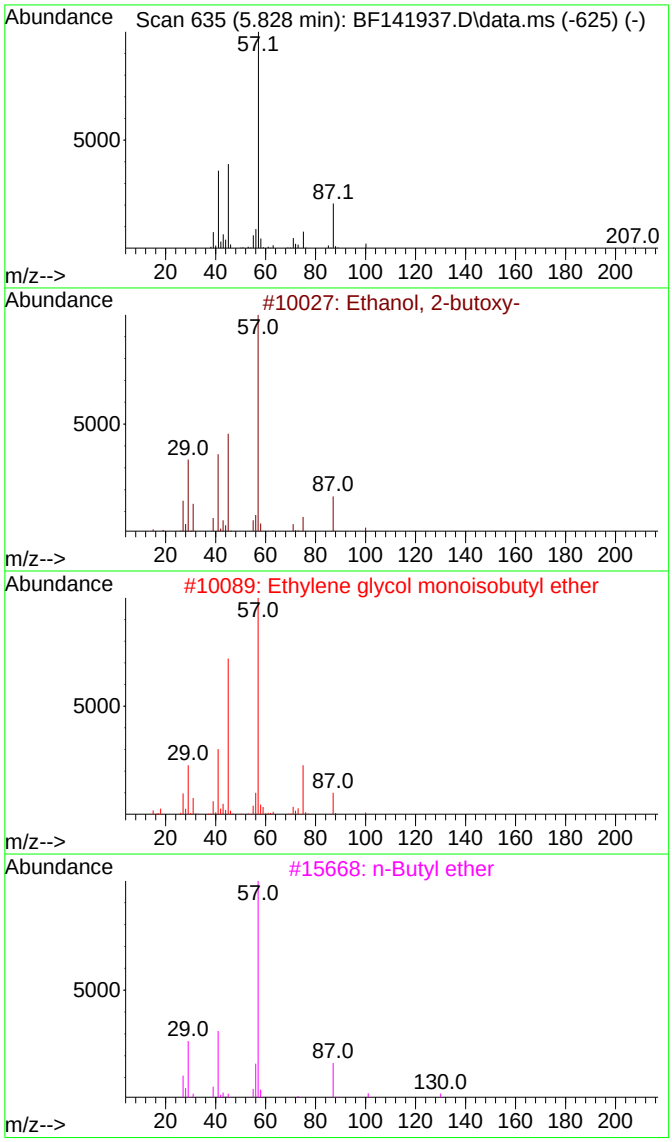
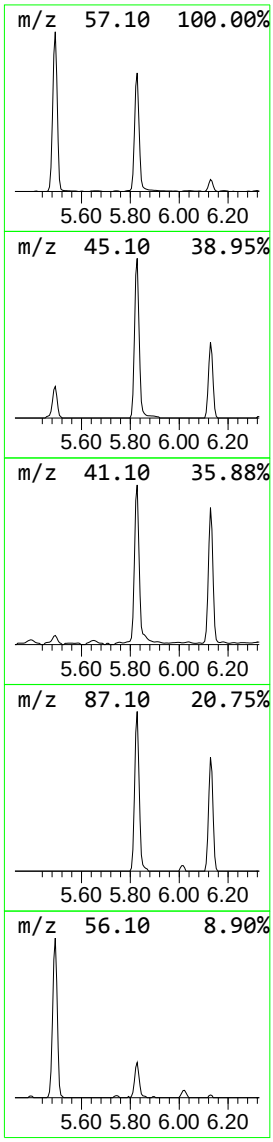
****

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	4.30 ng	201038	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3	n-Butyl ether	130	C8H18O	000142-96-1	25
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	25
5	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	25





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

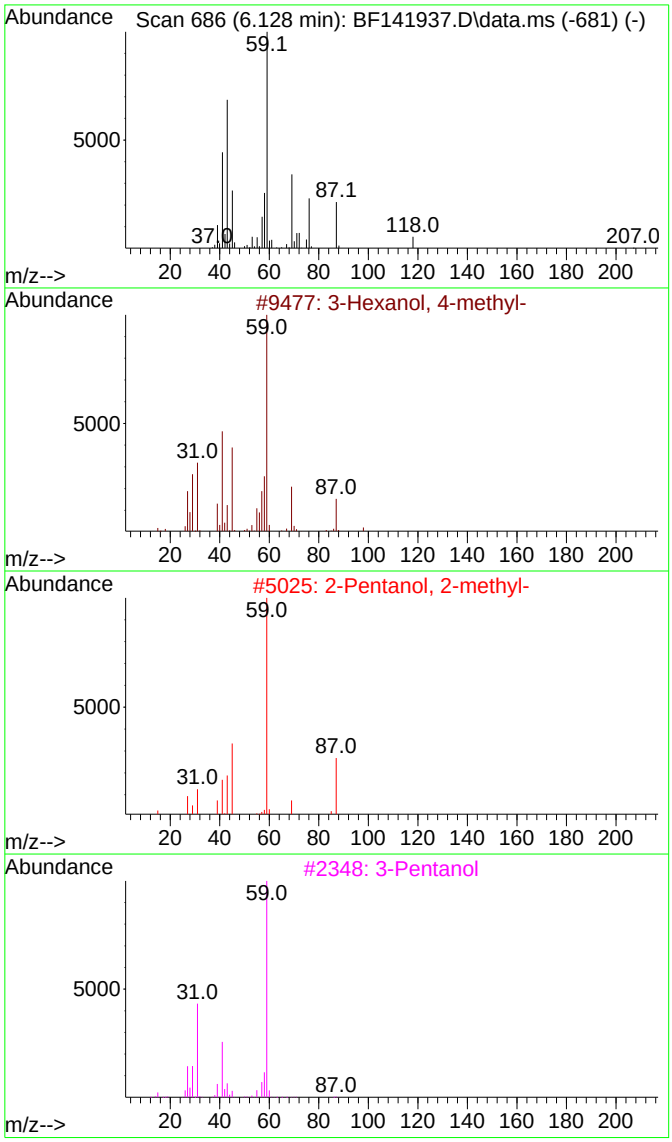
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

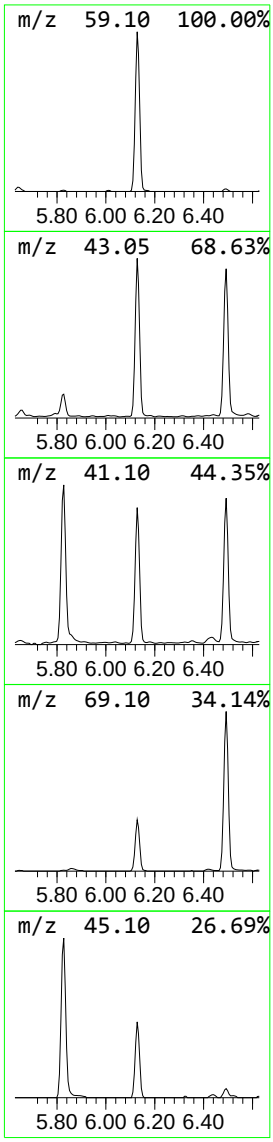
****

Peak Number 3 3-Hexanol, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.128	4.35 ng	203772	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	64
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
3	3-Pentanol	88	C5H12O	000584-02-1	43
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	40





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Acq On : 12 Mar 2025 14:26
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Sample : Q1522-02
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TIC Library : C:\Database\NIST20.L
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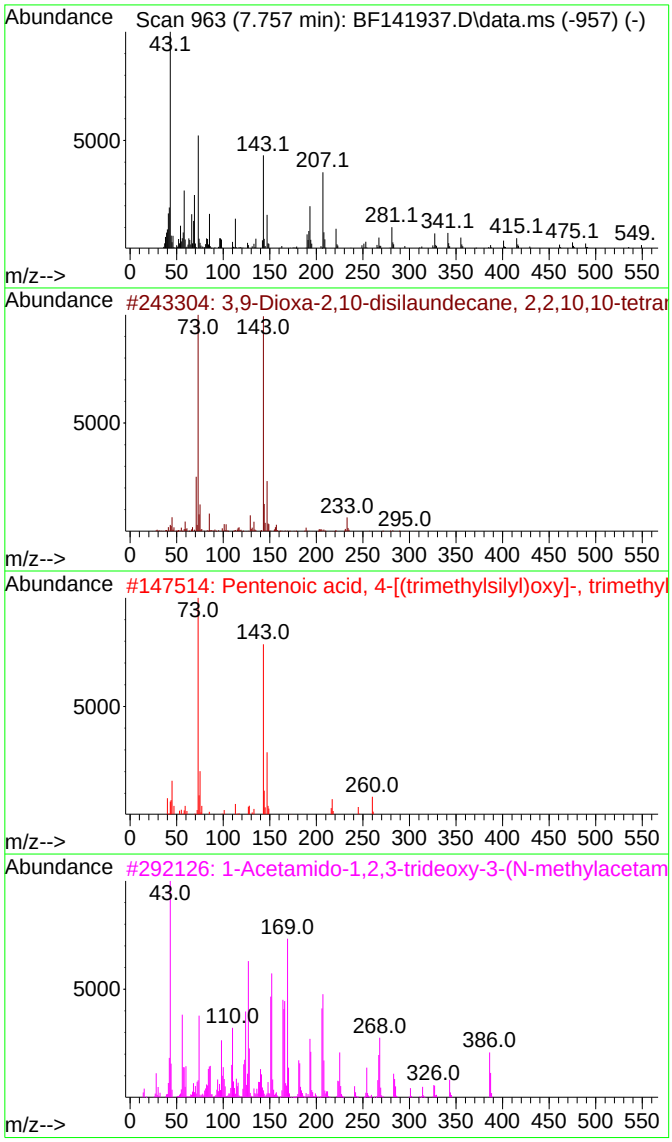
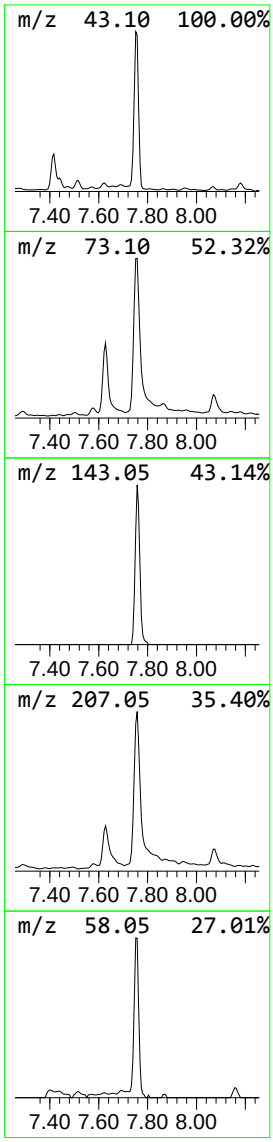
****

Peak Number 4 unknown7.757 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.757	6.81 ng	440267	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,9-Dioxa-2,10-disilaundecane, 2...	336	C14H36O3Si3	074685-22-6	22
2	Pentenoic acid, 4-[(trimethylsil...	260	C11H24O3Si2	072101-11-2	12
3	1-Acetamido-1,2,3-trideoxy-3-(N-...	386	C17H26N2O8	027425-84-9	12
4	2H-1,2,3-Triazol-4-amine, 2-meth...	143	C3H5N5O2	1000258-90-5	12
5	4-Hydroxypent-2-enoic acid, 2O-TMS	260	C11H24O3Si2	1000465-41-3	12





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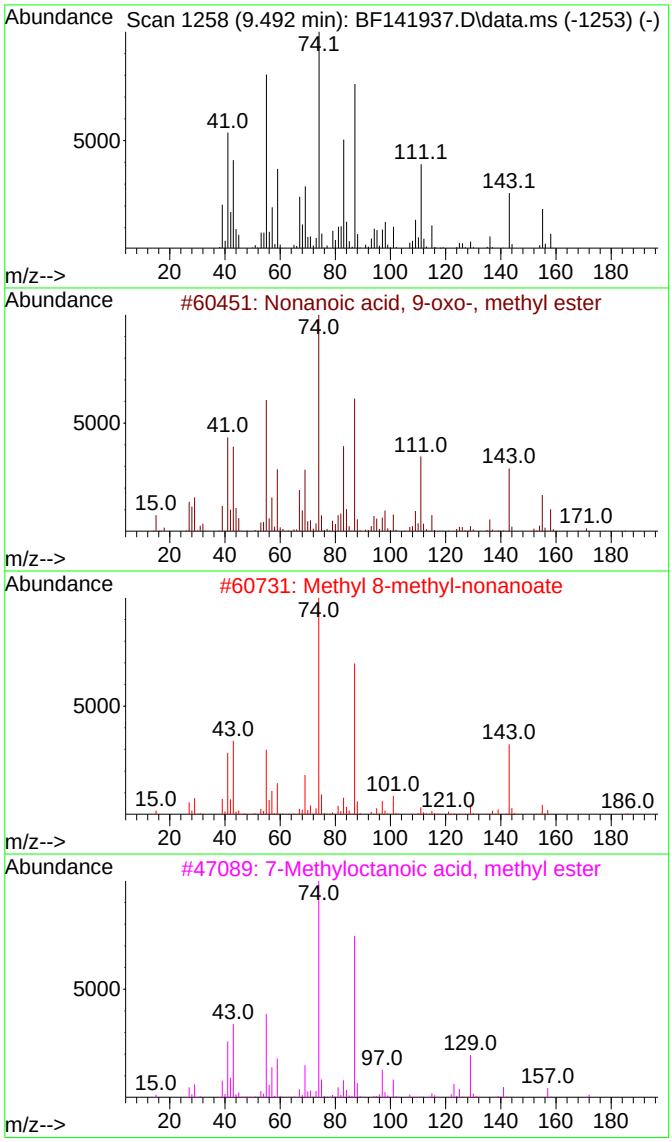
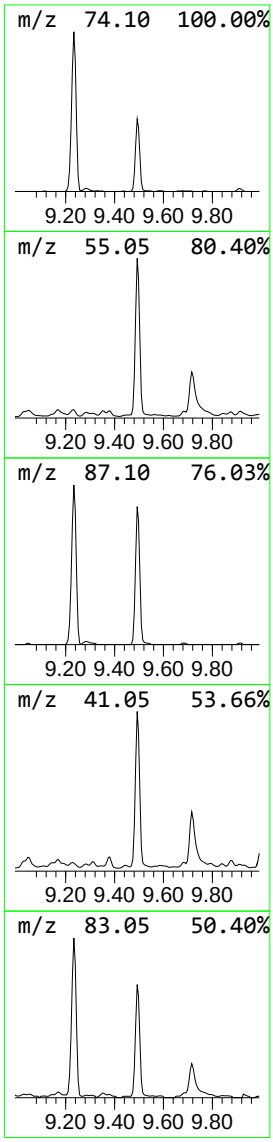
****
Peak Number 5 Nonanoic acid, 9-oxo-, meth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	4.27 ng	314453	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	91
2	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	50
3	7-Methyloctanoic acid, methyl ester	172	C10H20O2	005129-53-3	43
4	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	43
5	Octanoic acid, 8-hydroxy-, methy...	174	C9H18O3	020257-95-8	38





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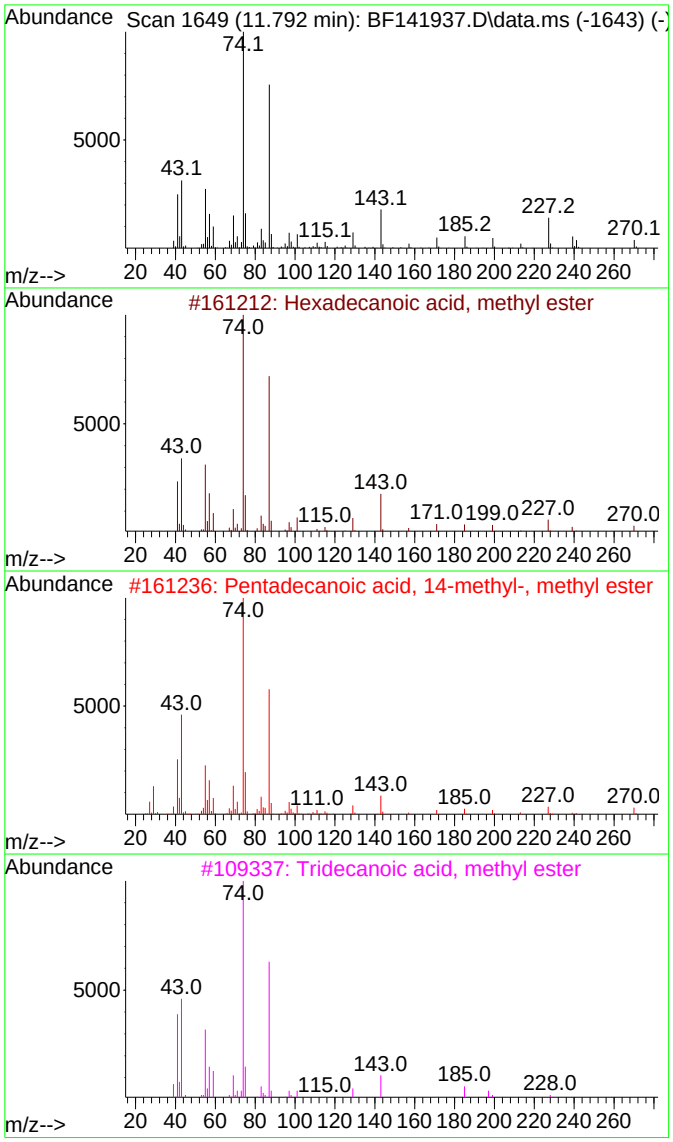
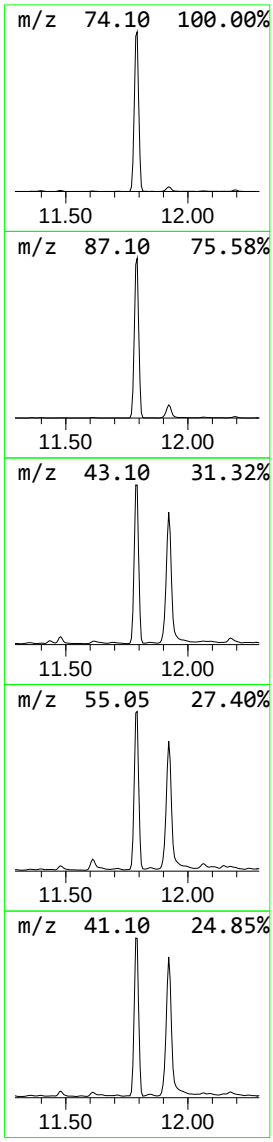
****
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	17.26 ng	1263910	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Misc :
ALS Vial : 8 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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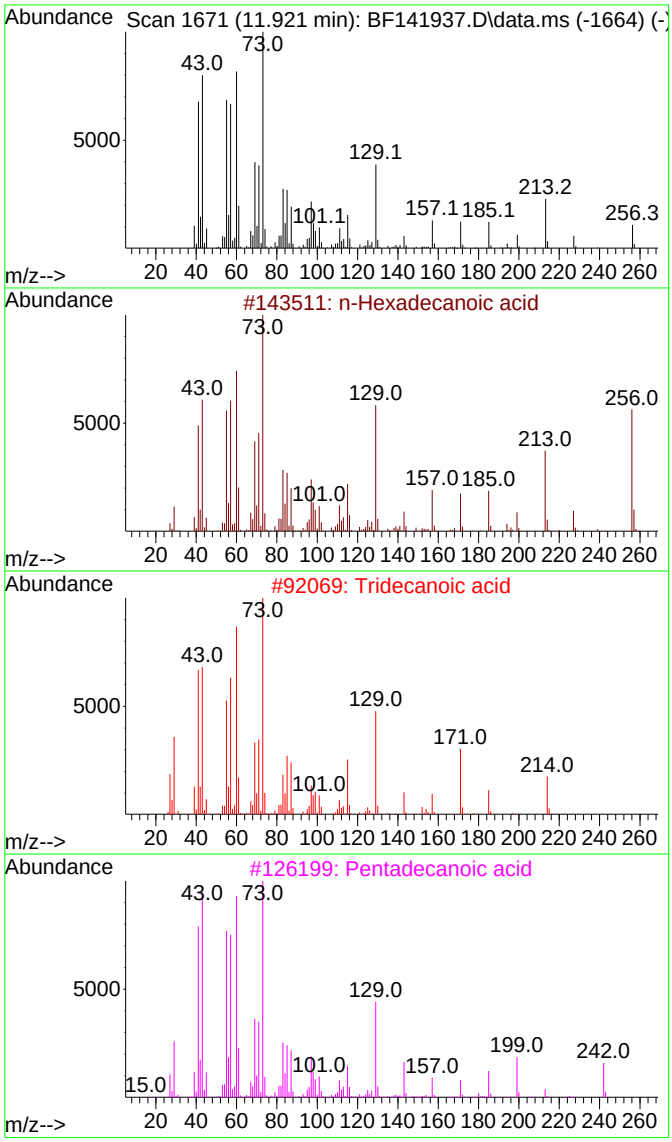
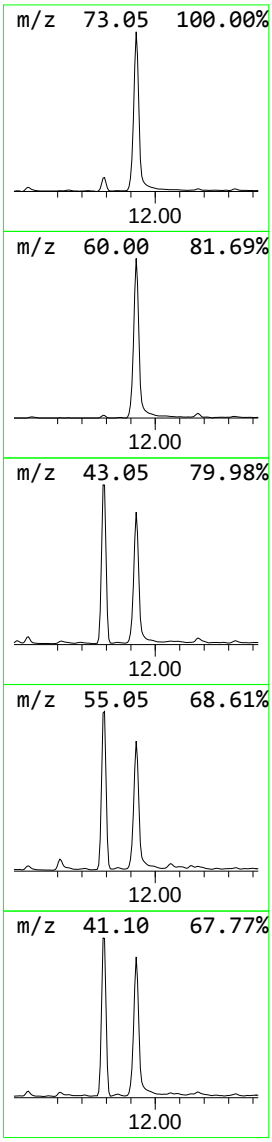
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	15.24 ng	1116340	Phenanthrene-d10	11.398

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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TIC Library : C:\Database\NIST20.L
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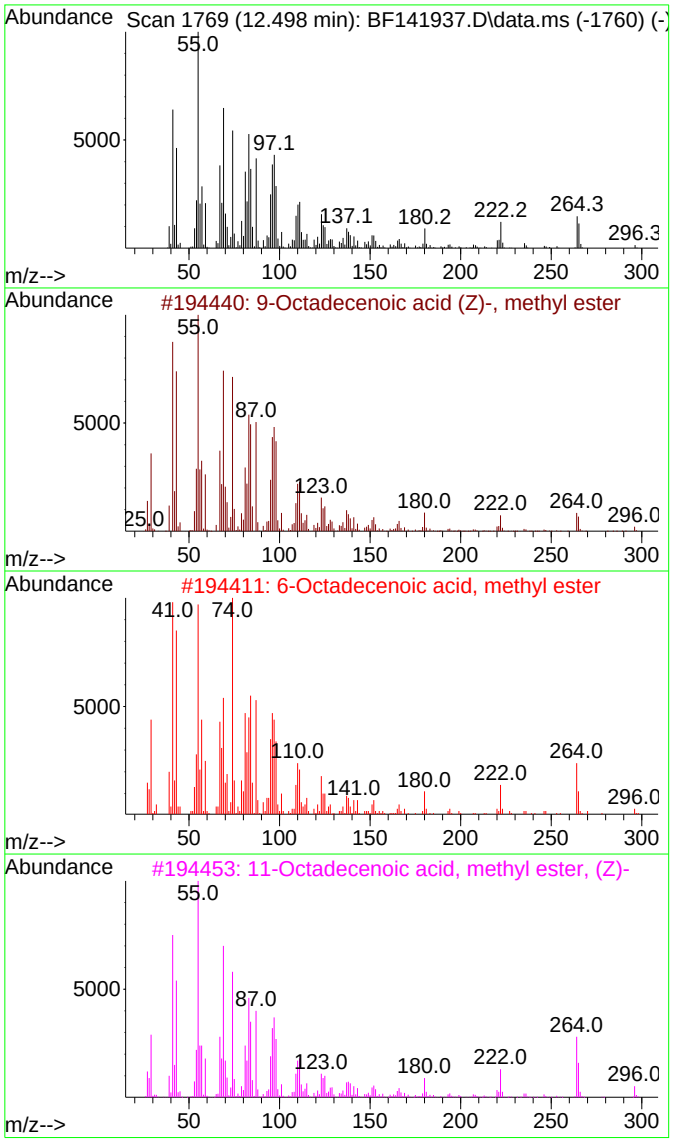
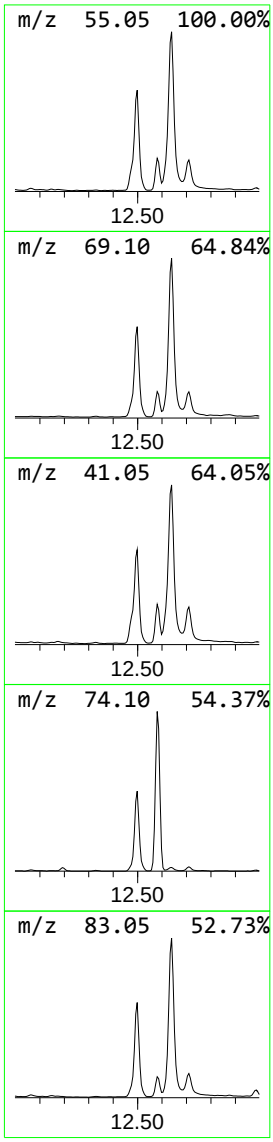
****
Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	23.68 ng	1734370	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99





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Data File : BF141937.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
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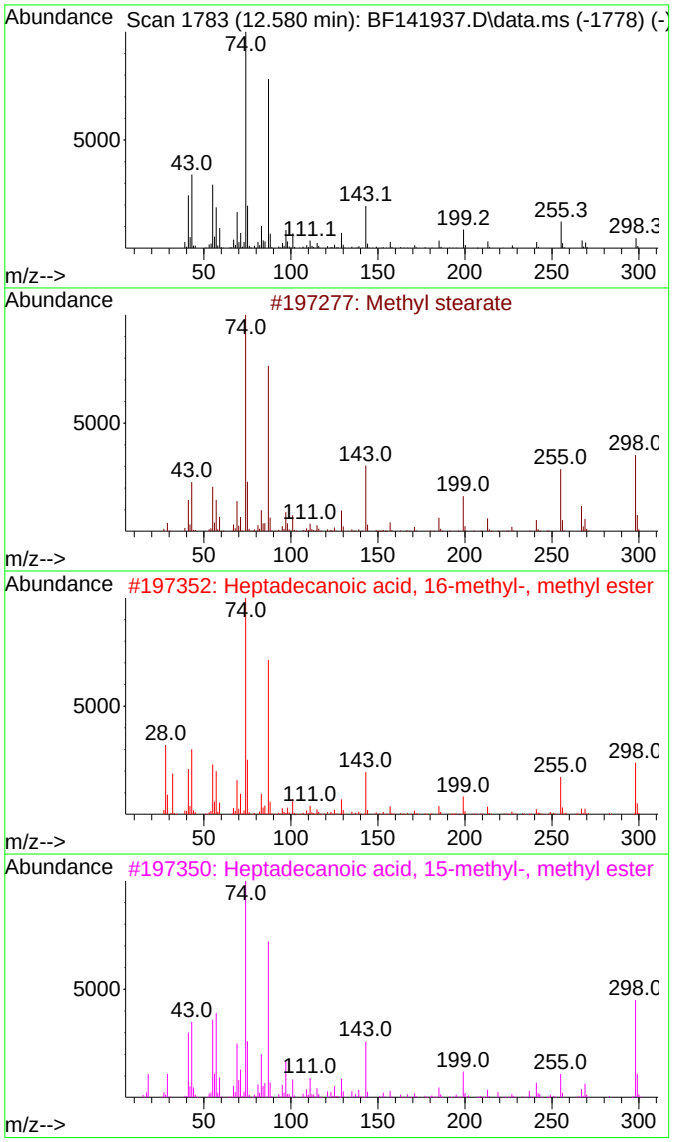
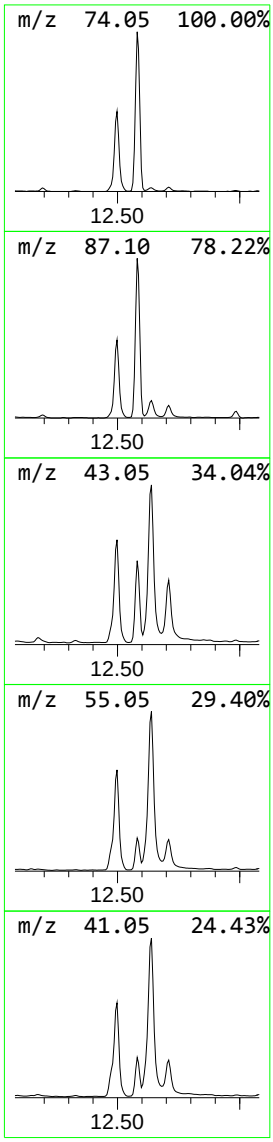
Peak Number 9 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	8.13 ng	595511	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
3	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Data File : BF141937.D
Acq On : 12 Mar 2025 14:26
Operator : RC/JU
Sample : Q1522-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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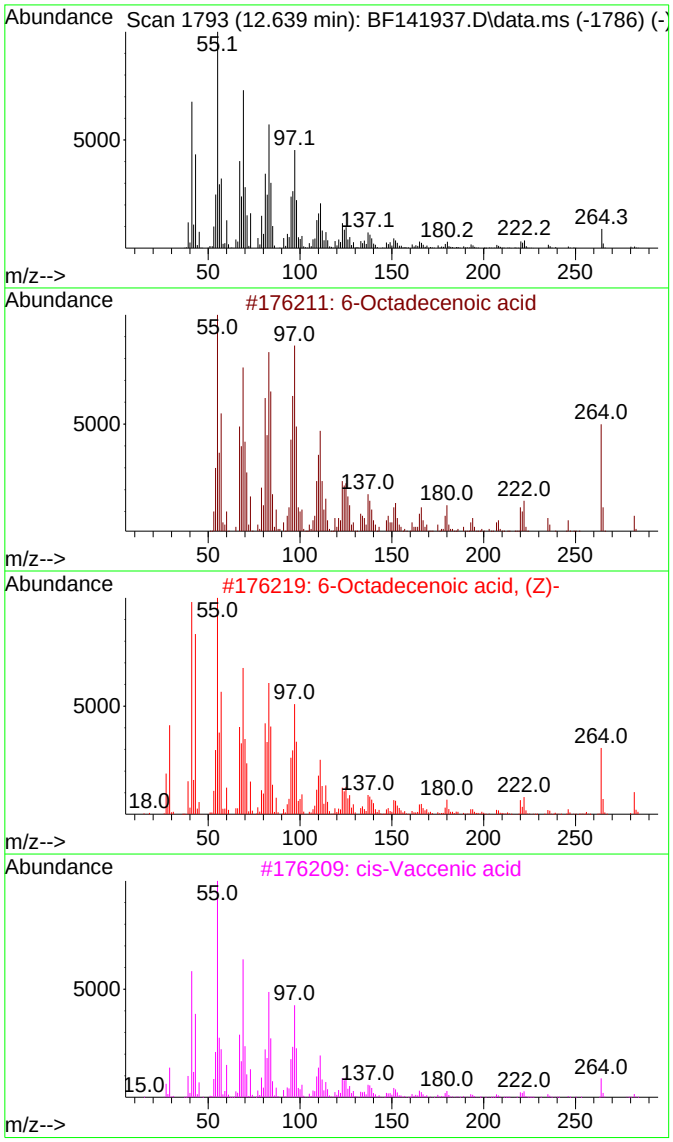
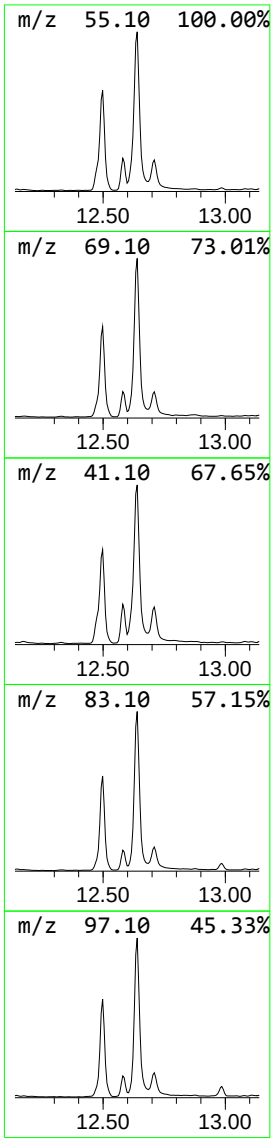
Peak Number 10 6-Octadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	36.47 ng	2670990	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	98
2	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	91
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
4	Oleic Acid	282	C18H34O2	000112-80-1	89
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87





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Data File : BF141937.D
Acq On : 12 Mar 2025 14:26
Operator : RC/JU
Sample : Q1522-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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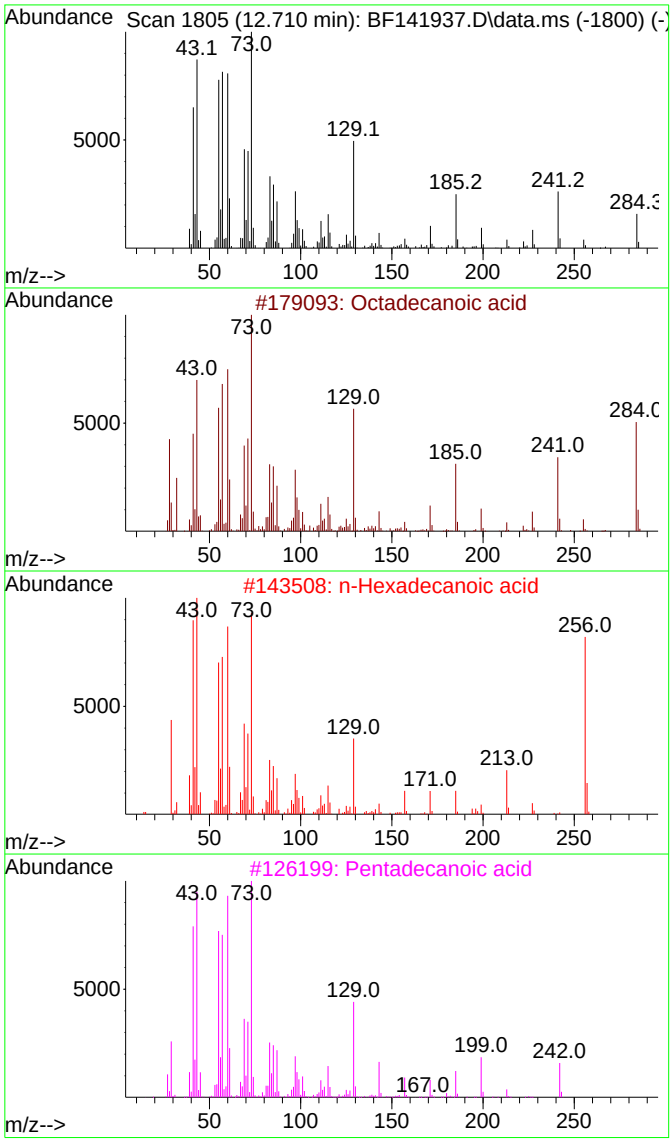
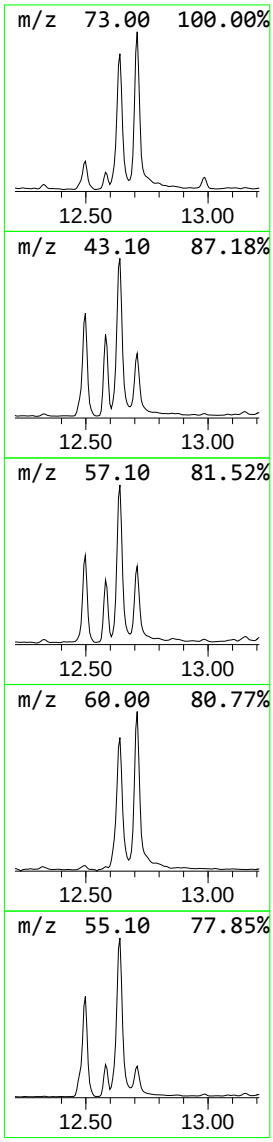
Peak Number 11 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	8.32 ng	608985	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Data File : BF141937.D
Acq On : 12 Mar 2025 14:26
Operator : RC/JU
Sample : Q1522-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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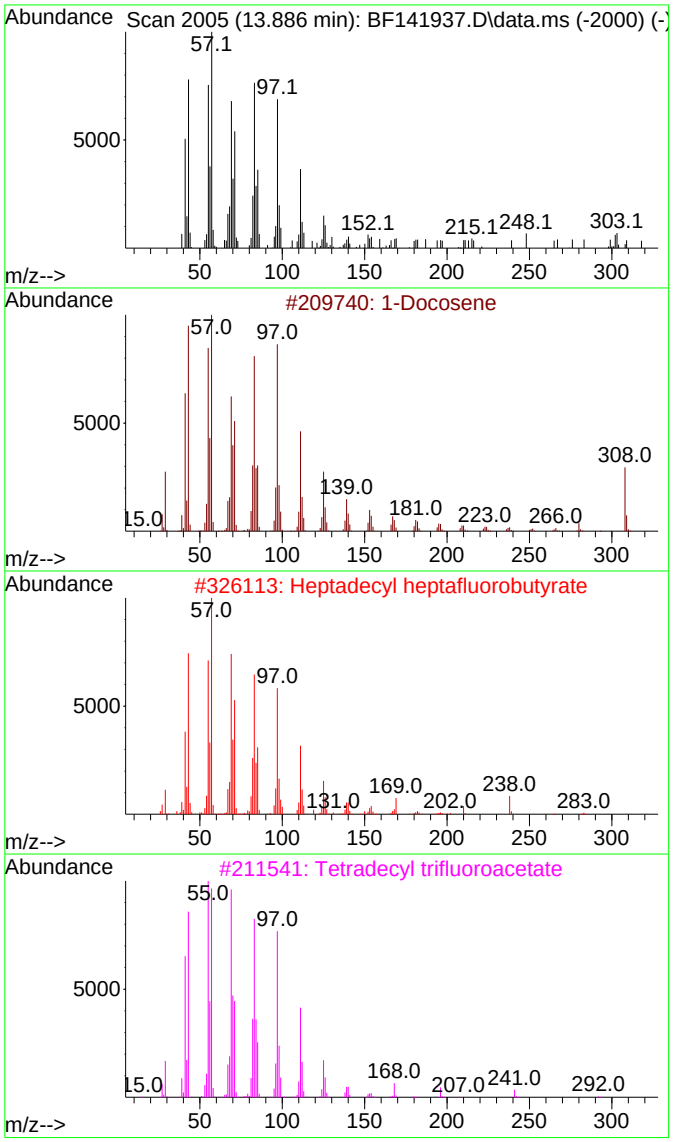
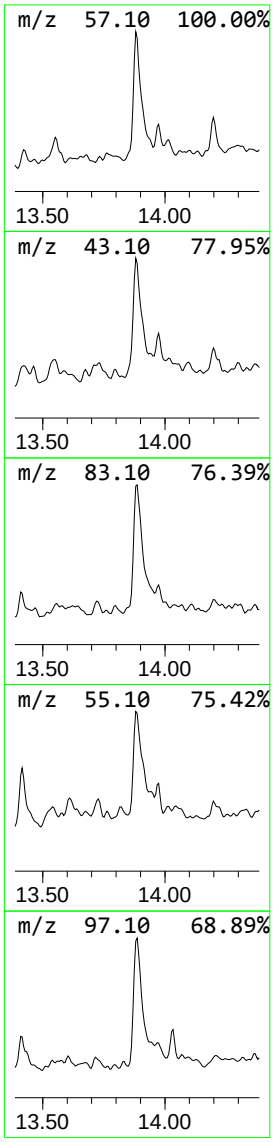
Peak Number 12 1-Docosene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.45 ng	119340	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	93
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5	Cyclopentadecane	210	C15H30	000295-48-7	89





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Data File : BF141937.D
Acq On : 12 Mar 2025 14:26
Operator : RC/JU
Sample : Q1522-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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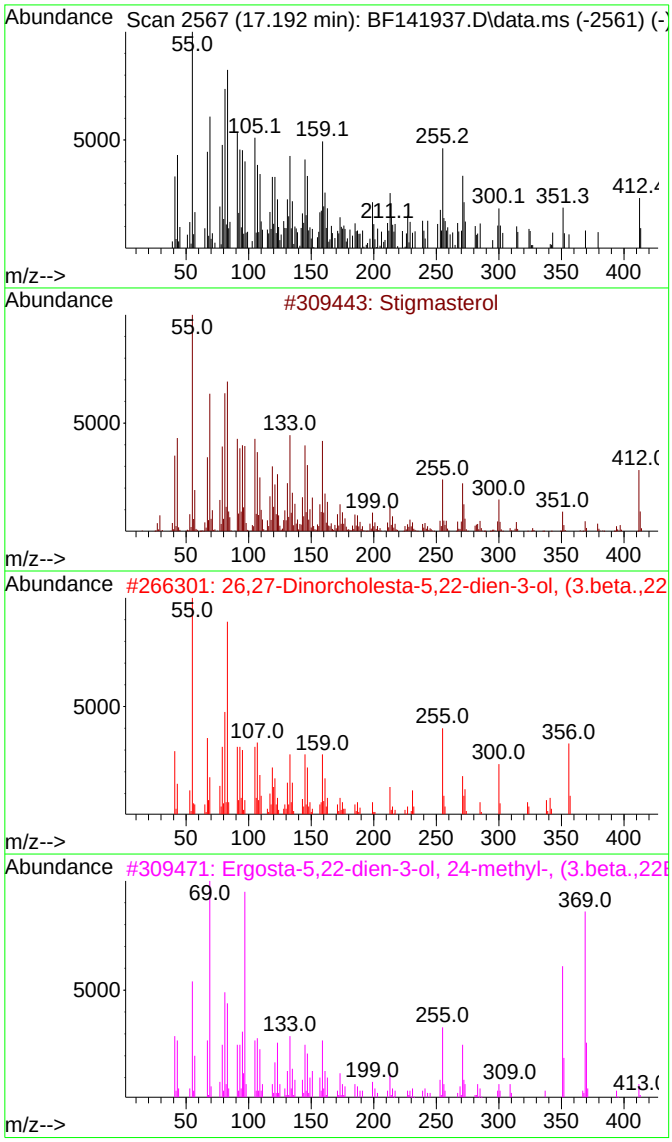
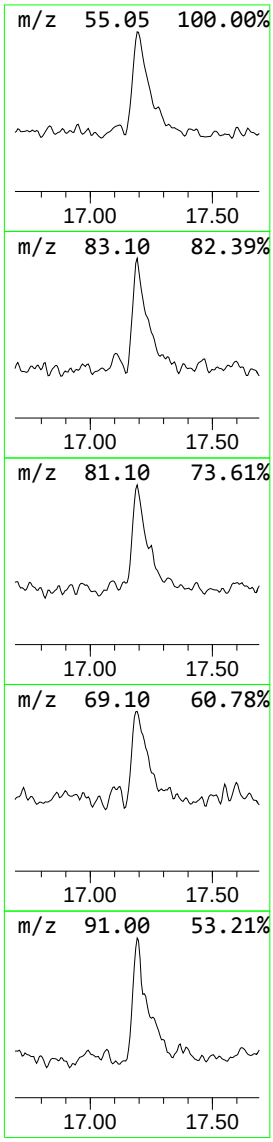
Peak Number 13 Stigmasterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.192	4.50 ng	211697	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	99
2	26,27-Dinorcholesta-5,22-dien-3-...	356	C25H40O	057597-10-1	78
3	Ergosta-5,22-dien-3-ol, 24-methy...	412	C29H48O	053755-22-9	59
4	Chondrillasterol	412	C29H48O	000481-17-4	49
5	Ursodeoxycholic acid	392	C24H40O4	000128-13-2	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031225\
Data File : BF141937.D
Acq On : 12 Mar 2025 14:26
Operator : RC/JU
Sample : Q1522-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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...	2.175	107.0	ng	5008730	1	6.881	936009	20.0
Ethanol, 2-butoxy-	5.828	4.3	ng	201038	1	6.881	936009	20.0
3-Hexanol, 4-me...	6.128	4.3	ng	203772	1	6.881	936009	20.0
unknown7.757	7.757	6.8	ng	440267	2	8.157	1293770	20.0
Nonanoic acid, ...	9.492	4.3	ng	314453	3	9.910	1473550	20.0
Hexadecanoic ac...	11.792	17.3	ng	1263910	4	11.398	1464630	20.0
n-Hexadecanoic ...	11.922	15.2	ng	1116340	4	11.398	1464630	20.0
9-Octadecenoic ...	12.498	23.7	ng	1734370	4	11.398	1464630	20.0
Methyl stearate	12.580	8.1	ng	595511	4	11.398	1464630	20.0
6-Octadecenoic ...	12.639	36.5	ng	2670990	4	11.398	1464630	20.0
Octadecanoic acid	12.710	8.3	ng	608985	4	11.398	1464630	20.0
1-Docosene	13.886	2.5	ng	119340	5	14.033	975226	20.0
Stigmasterol	17.192	4.5	ng	211697	6	15.509	941191	20.0