LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RVE-168

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	471	474	491	rVB	146293	171634	5.24%	0.655%
2	5.487	540	544	557	rVB	3426723	3014321	91.98%	11.506%
3	6.504	712	717	729	rVB	2981078	2964399	90.46%	11.316%
4	6.845	772	775	779	rBV	1138195	900677	27.48%	3.438%
5	7.410	866	871	874	rBV	2041577	1888293	57.62%	7.208%
6	8.128	989	993	996	rBV	1352809	1100032	33.57%	4.199%
7	9.204	1171	1176	1179	rBV	3884347	3277101	100.00%	12.509%
8	9.463	1216	1220	1224	rBV	64385	55173	1.68%	0.211%
9	9.886	1288	1292	1295	rVB	1234355	1091307	33.30%	4.166%
10	10.675	1422	1426	1430	rBV	2010626	1880718	57.39%	7.179%
11	10.786	1440	1445	1453	rVB5	38930	71259	2.17%	0.272%
12	11.375	1541	1545	1547	rBV	1277860	1032241	31.50%	3.940%
13	11.398	1547	1549	1554	rVB	91531	82206	2.51%	0.314%
14	11.604	1580	1584	1587	rBV4	26977	41193	1.26%	0.157%
15	11.751	1606	1609	1613	rVB	178920	140975	4.30%	0.538%
16	11.892	1631	1633	1637	rVB2	93672	112383	3.43%	0.429%
17	11.986	1645	1649	1651	rBV2	40814	41074	1.25%	0.157%
18	12.422	1720	1723	1725	rBV	52401	52848	1.61%	0.202%
19	12.457	1725	1729	1732	rVB2	149850	143805	4.39%	0.549%
20	12.545	1741	1744	1748	rVB	57406	43369	1.32%	0.166%
21	12.586	1748	1751	1754	rBV	213106	173211	5.29%	0.661%
22	12.816	1785	1790	1797	rBV	204281	240795	7.35%	0.919%
23	12.957	1810	1814	1818	rVB	3361266	2923646	89.21%	11.160%
24	13.033	1824	1827	1834	rBV5	23279	39181	1.20%	0.150%
25	13.174	1848	1851	1855	rVB	45130	40428	1.23%	0.154%
26	13.516	1907	1909	1913	rBV2	44564	42237	1.29%	0.161%
27	13.633	1927	1929	1931	rBV2	45207	42610	1.30%	0.163%
28	13.657	1931	1933	1938	rVB2	44231	49180	1.50%	0.188%
29	13.851	1962	1966	1978	rVB3	176846	374848	11.44%	1.431%
30	14.021	1990	1995	1997	rBV	972332	936423	28.57%	3.574%
31	14.045	1997	1999	2001	rVB	90141	65196	1.99%	0.249%
32	14.110	2006	2010	2014	rBV	373585	353815	10.80%	1.351%
33	14.163	2016	2019	2021	rBV	73045	60489	1.85%	0.231%
34	14.286	2038	2040	2045	rVB3	55203	53947	1.65%	0.206%
35	14.468	2068	2071	2073	rBV	151920	137241	4.19%	0.524%
36	14.768	2120	2122	2125	rVB	93436	87950	2.68%	0.336%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.845	2133	2135	2138	rVB	75811	69734	2.13%	0.266%
38	14.915	2145	2147	2152	rVB	126404	131250	4.01%	0.501%
39	15.063	2169	2172	2175	rBV	68735	100866	3.08%	0.385%
40	15.110	2176	2180	2184	rVB	222755	271132	8.27%	1.035%
41	15.492	2240	2245	2250	rBV	618594	823577	25.13%	3.144%
42	15.692	2275	2279	2287	rVB	145738	190845	5.82%	0.728%
43	15.921	2313	2318	2324	rVB	264564	391020	11.93%	1.493%
44	16.721	2449	2454	2460	rVB	274189	492990	15.04%	1.882%

Sum of corrected areas: 26197619

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
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Acq On : 06 Aug 2022 01:45
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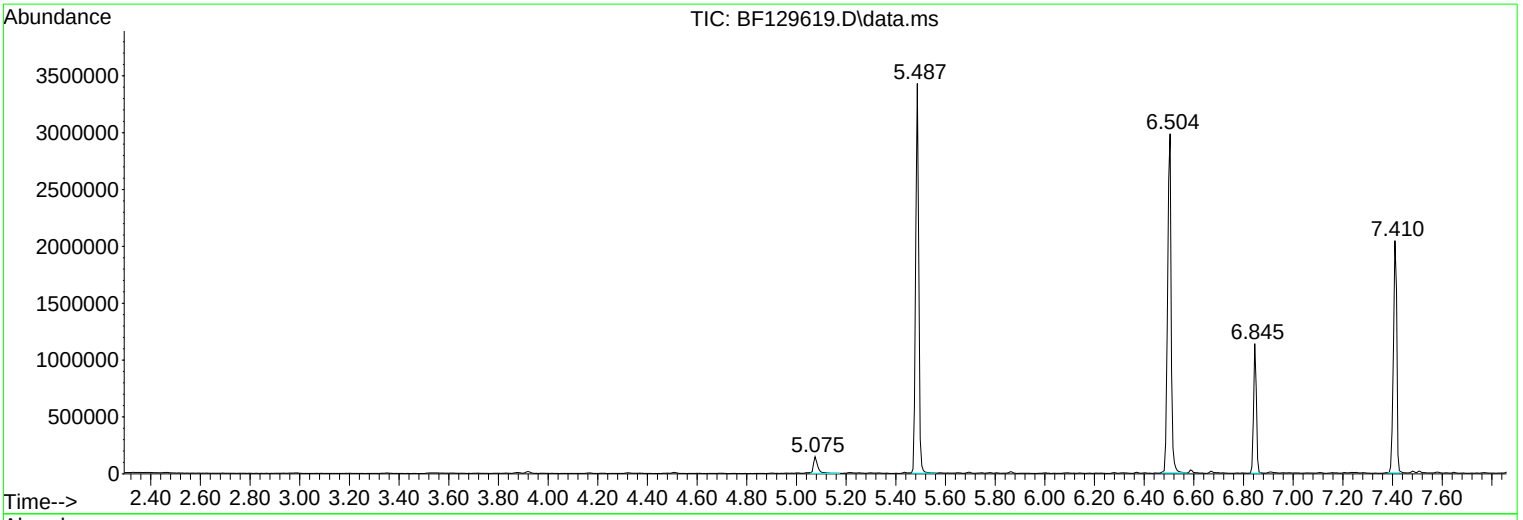
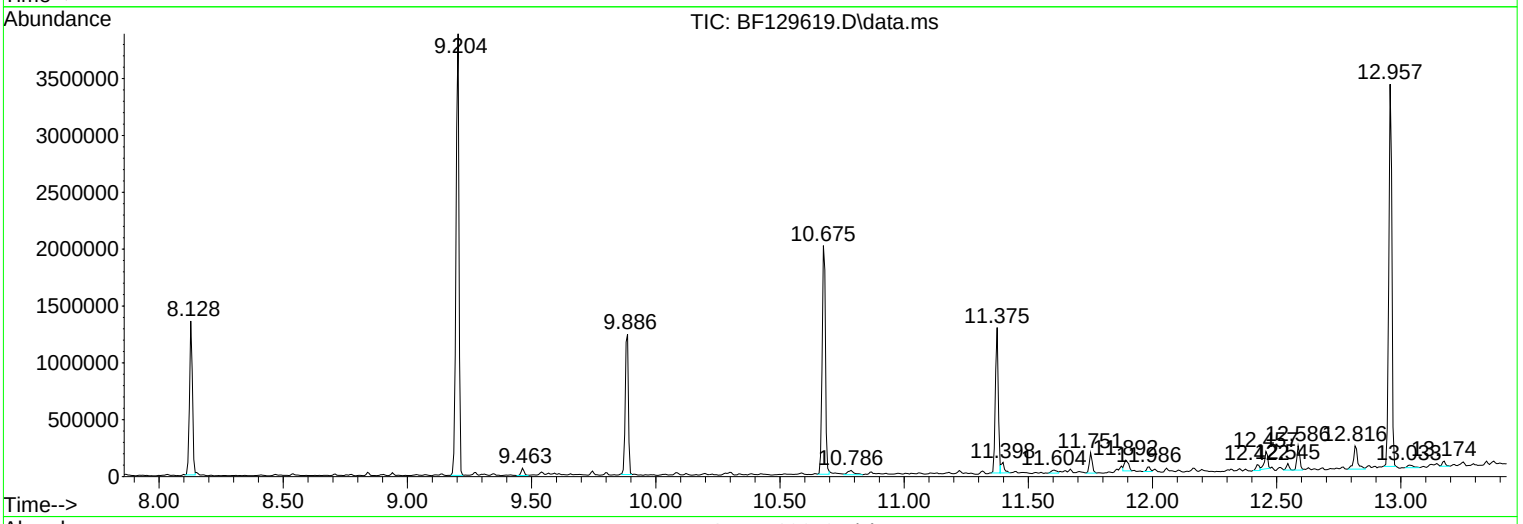
Misc :
ALS Vial : 16 Sample Multiplier: 1

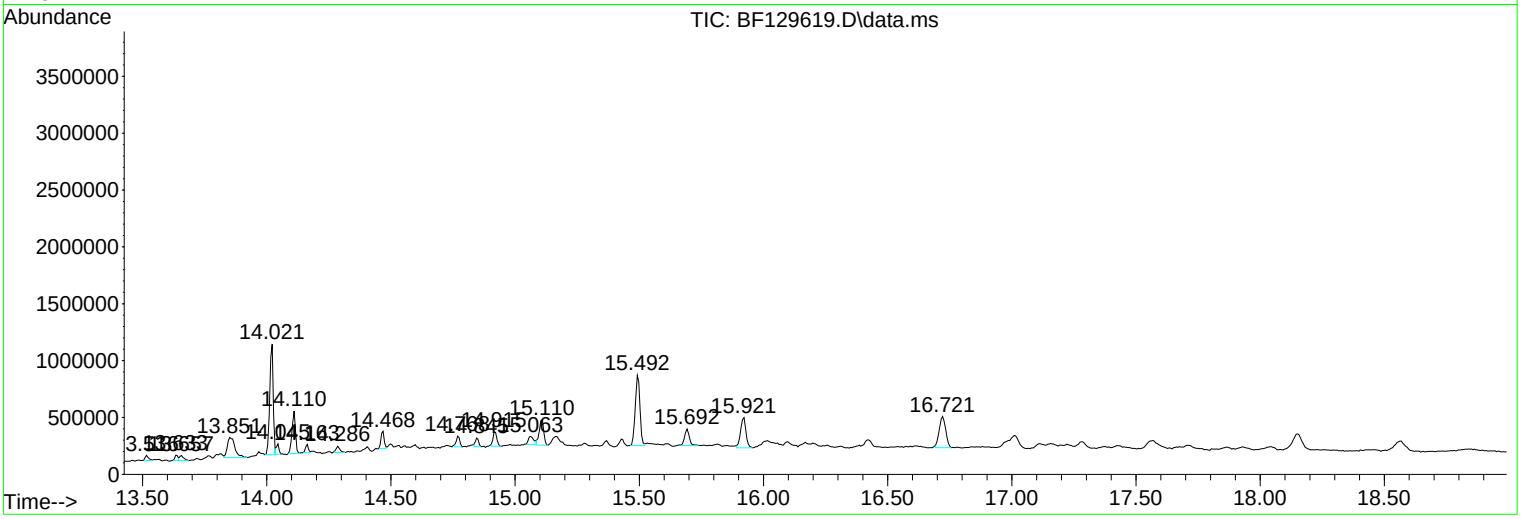
Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

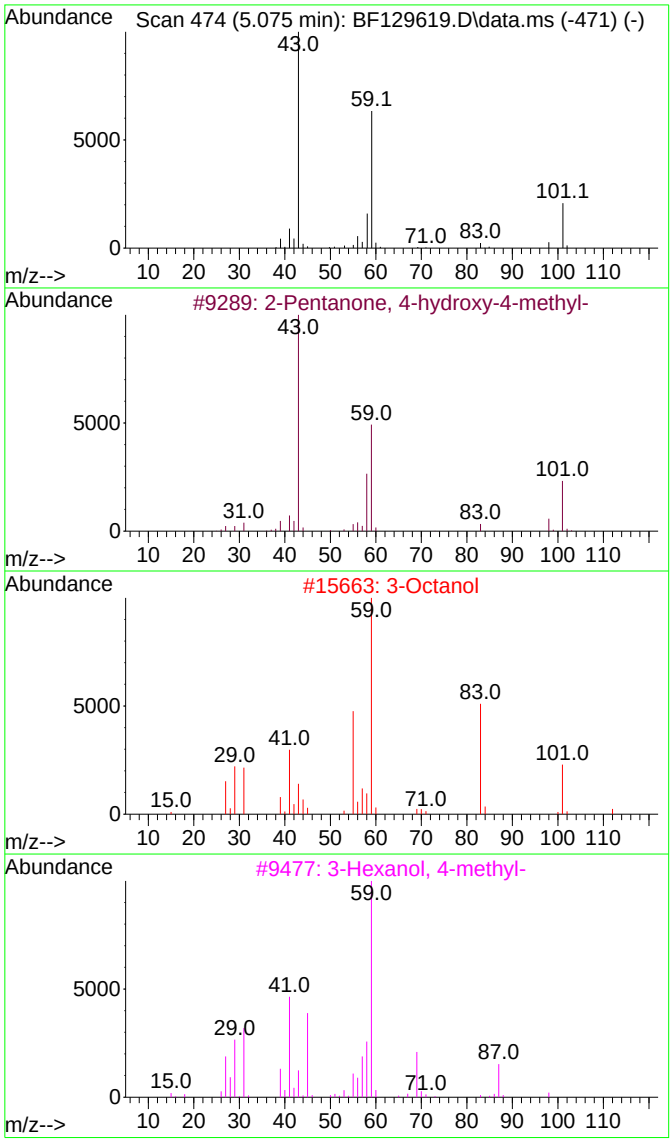
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

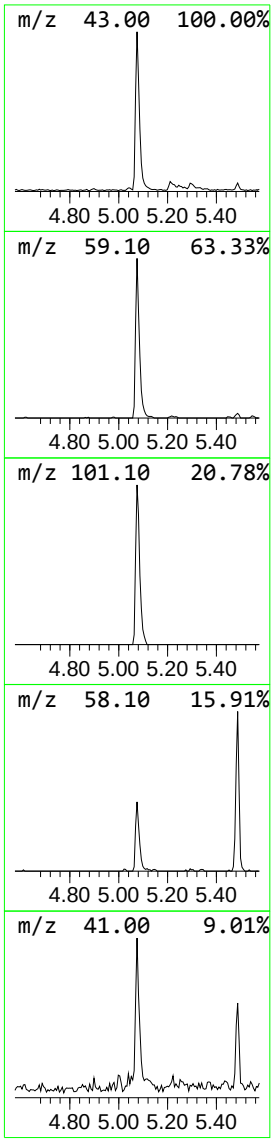
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.81 ng	171634	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Octanol	130	C8H18O	000589-98-0	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
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Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

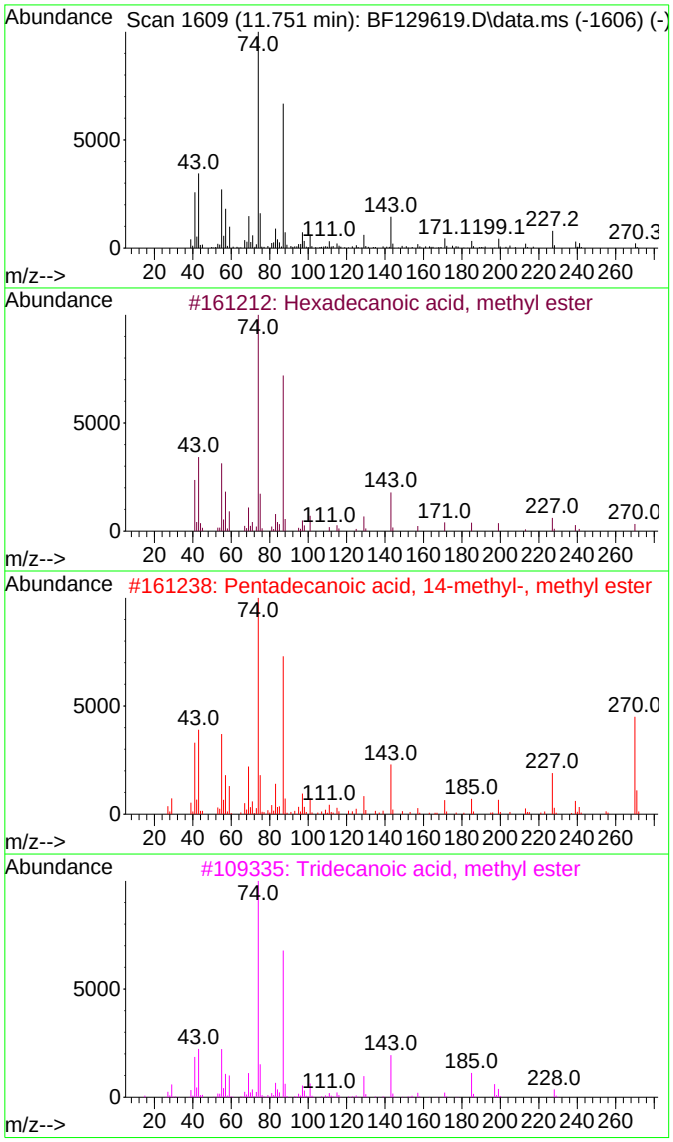
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

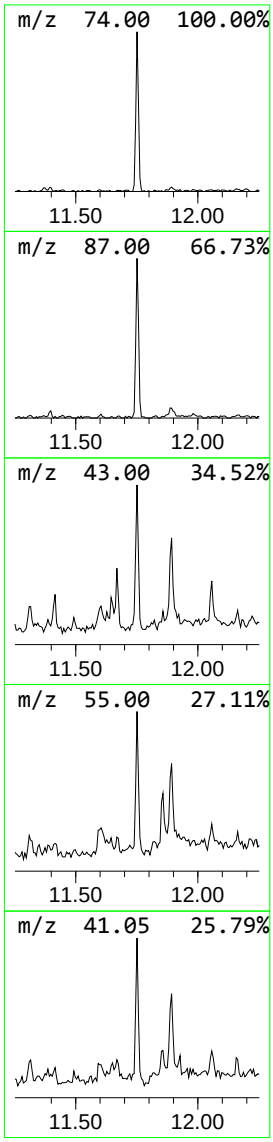
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.751	2.73 ng	140975	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

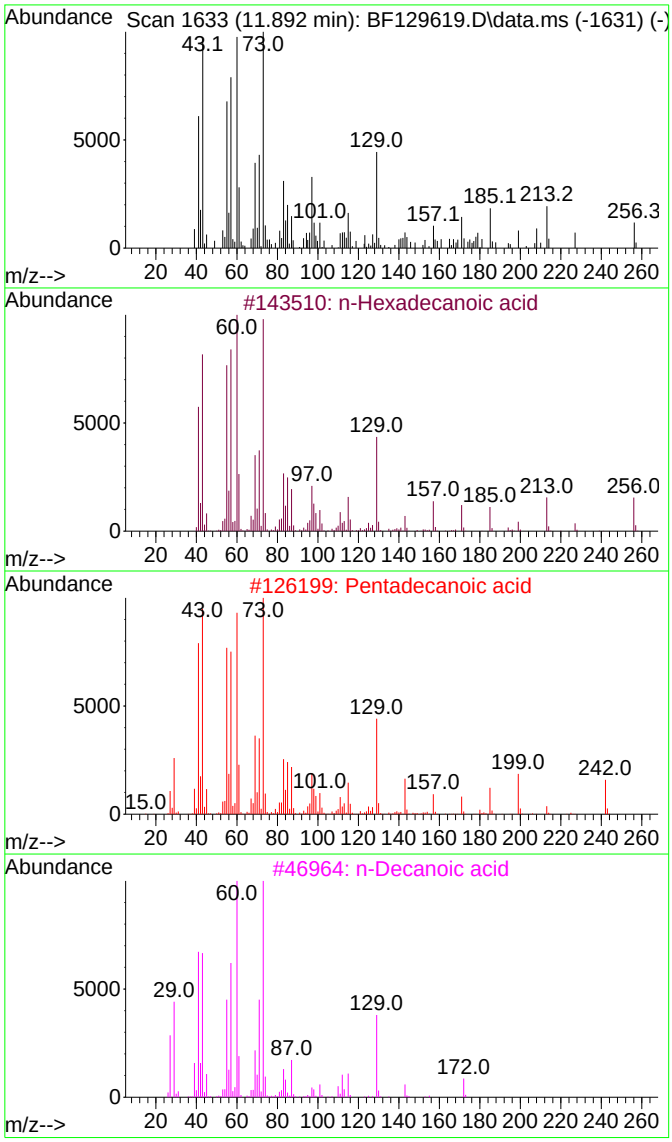
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

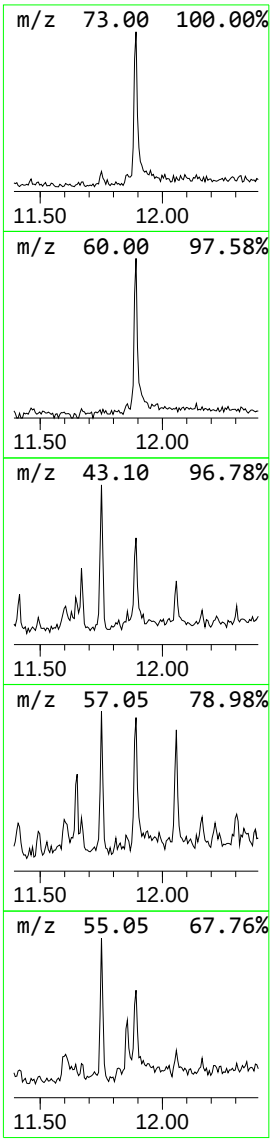
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.18 ng	112383	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	62
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

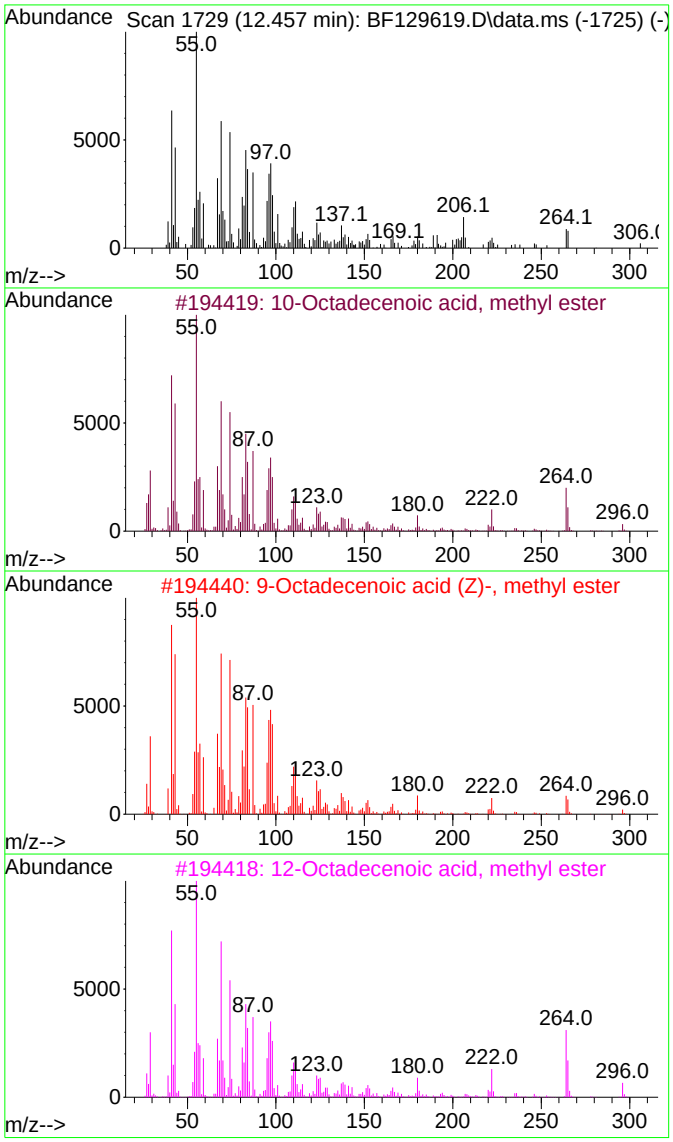
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

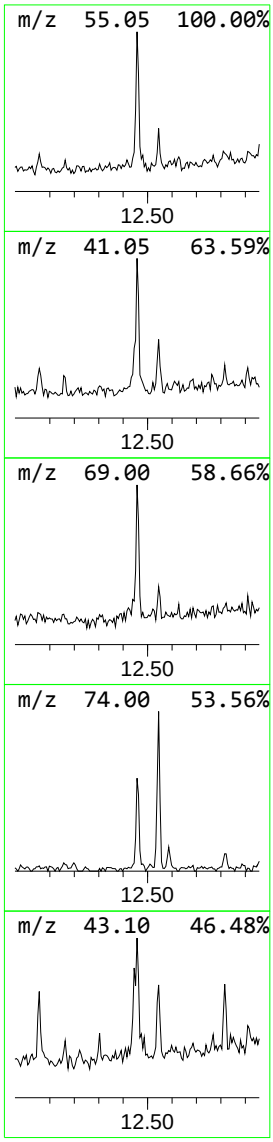
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	2.79 ng	143805	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	91
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

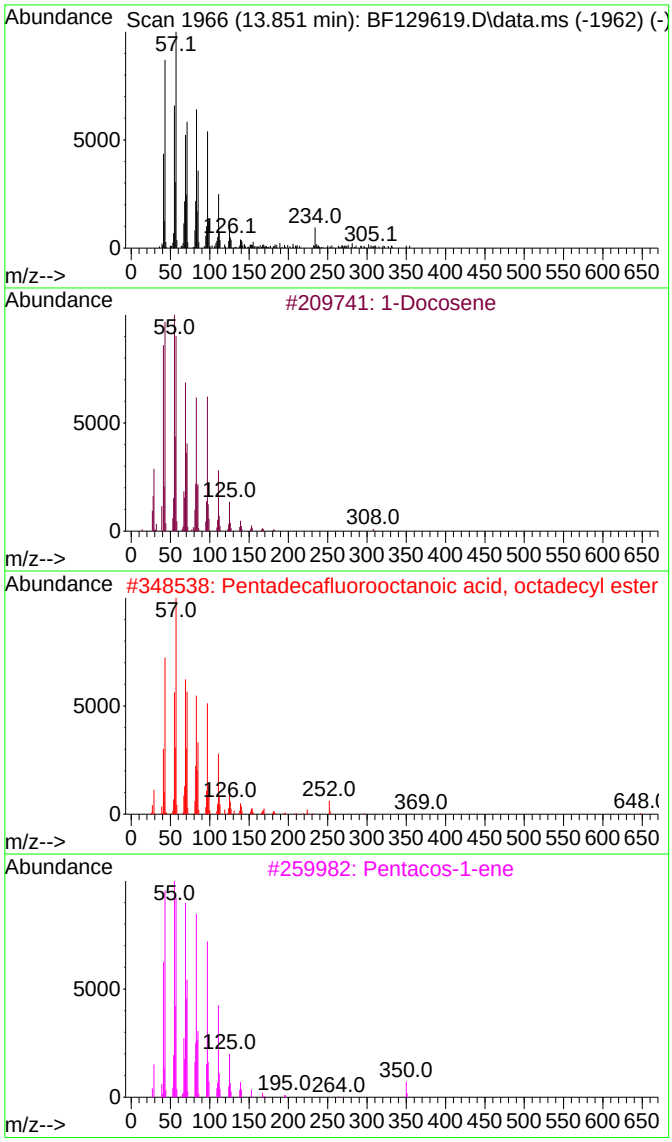
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

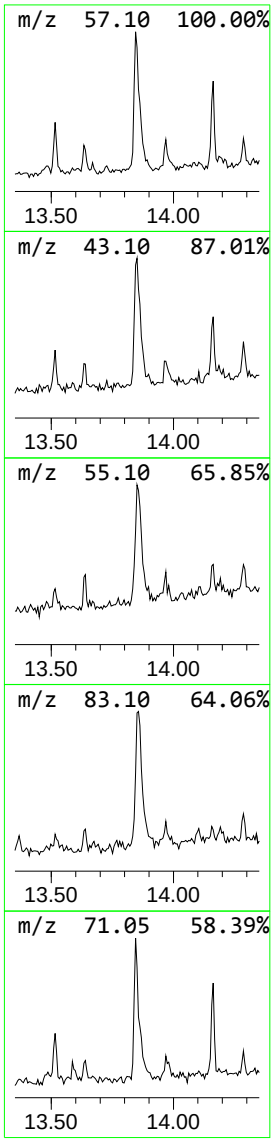
****

Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	8.01 ng	374848	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3	Pentacos-1-ene	350	C25H50	016980-85-1	93
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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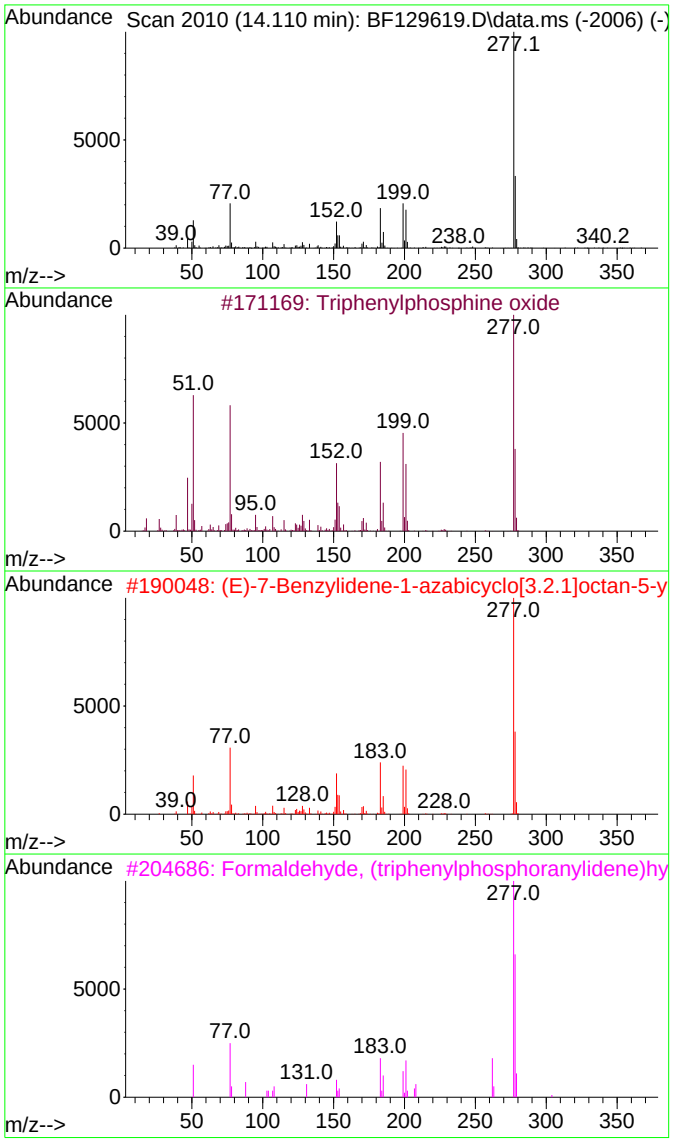
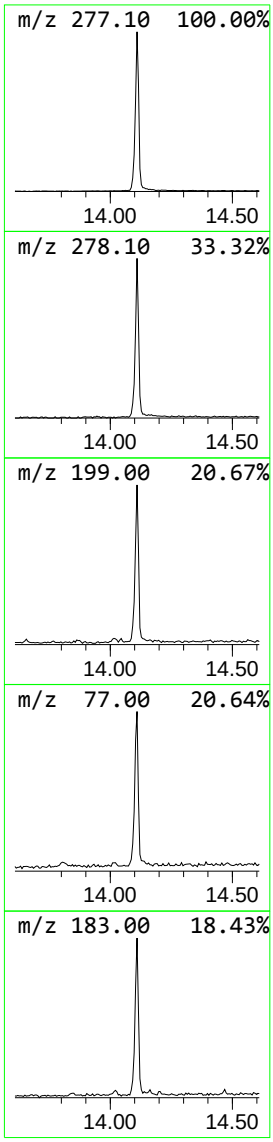
Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	7.56 ng	353815	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	76
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	37
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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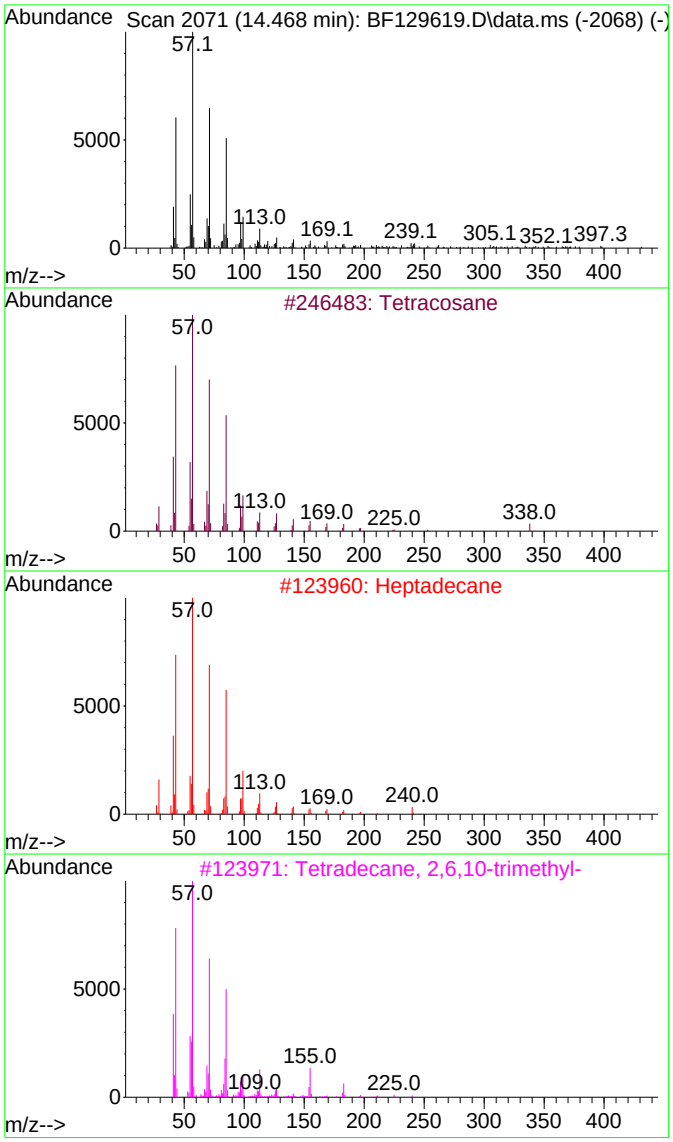
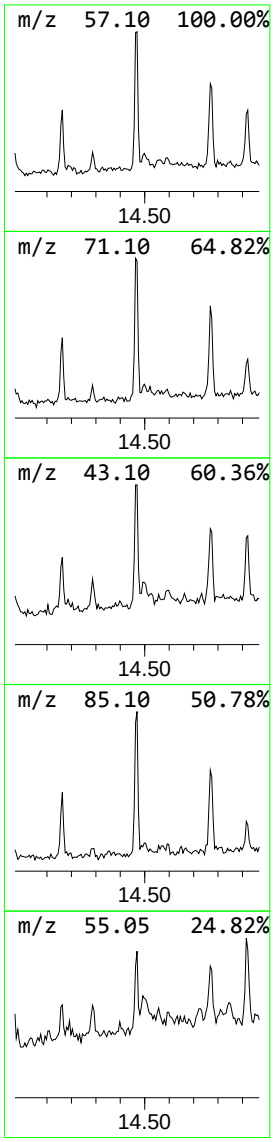
Peak Number 7 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.469	2.93 ng	137241	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	99
2	Heptadecane	240	C17H36	000629-78-7	96
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
5	9-Methylheneicosane	310	C22H46	070475-51-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

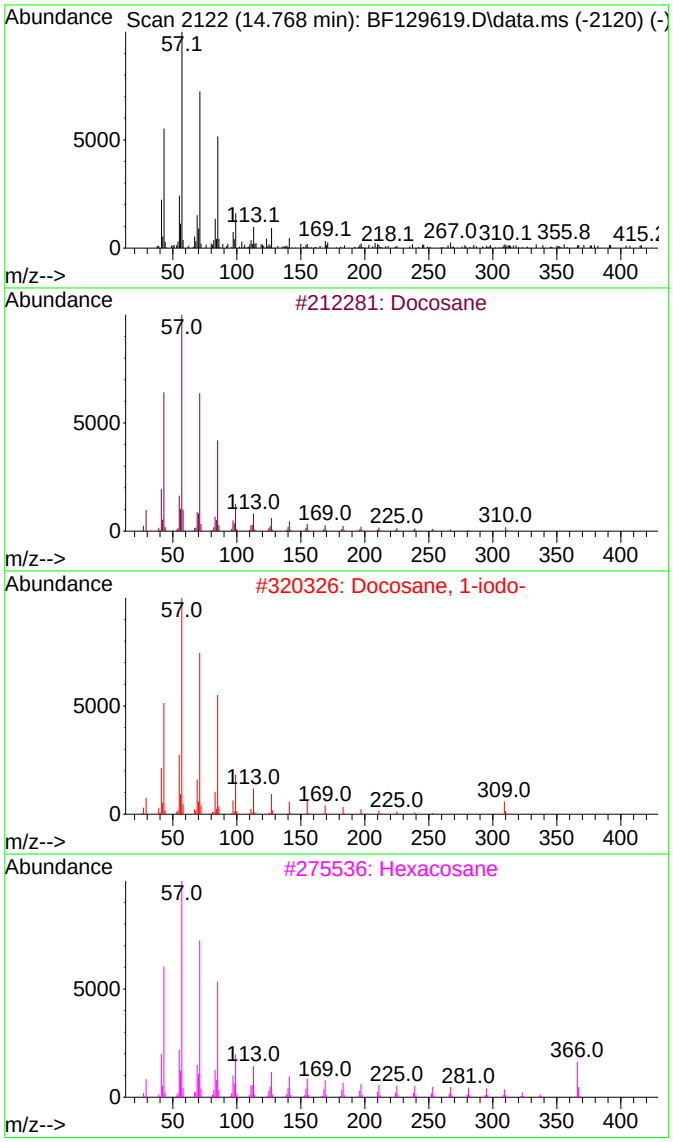
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

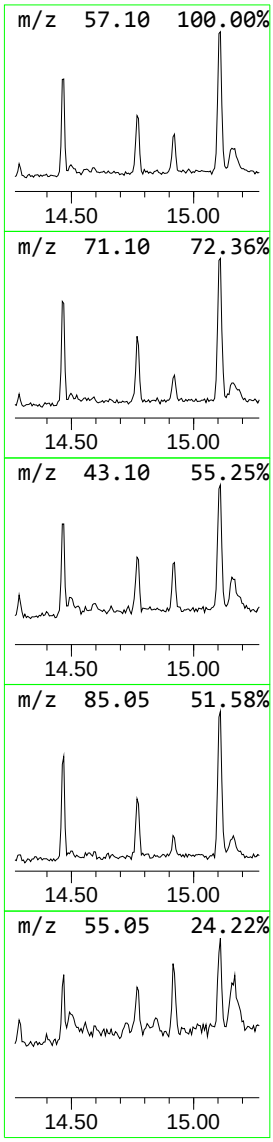
****

Peak Number 8 Docosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	2.14 ng	87950	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	81
3	Hexacosane	366	C26H54	000630-01-3	81
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	74
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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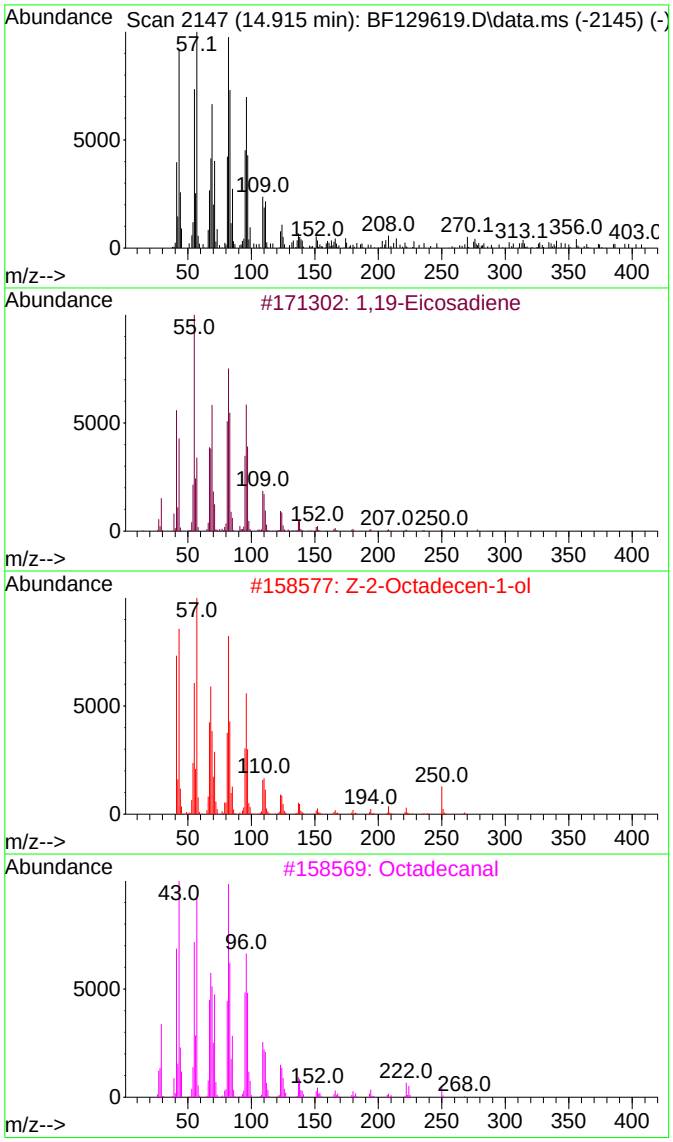
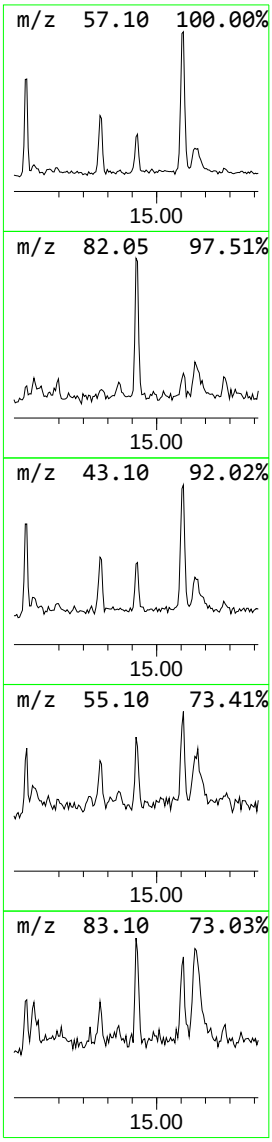
Peak Number 9 1,19-Eicosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	3.19 ng	131250	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	93
2	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Tetradecanal	212	C14H28O	000124-25-4	90
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68





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Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
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TIC Library : C:\Database\NIST20.L
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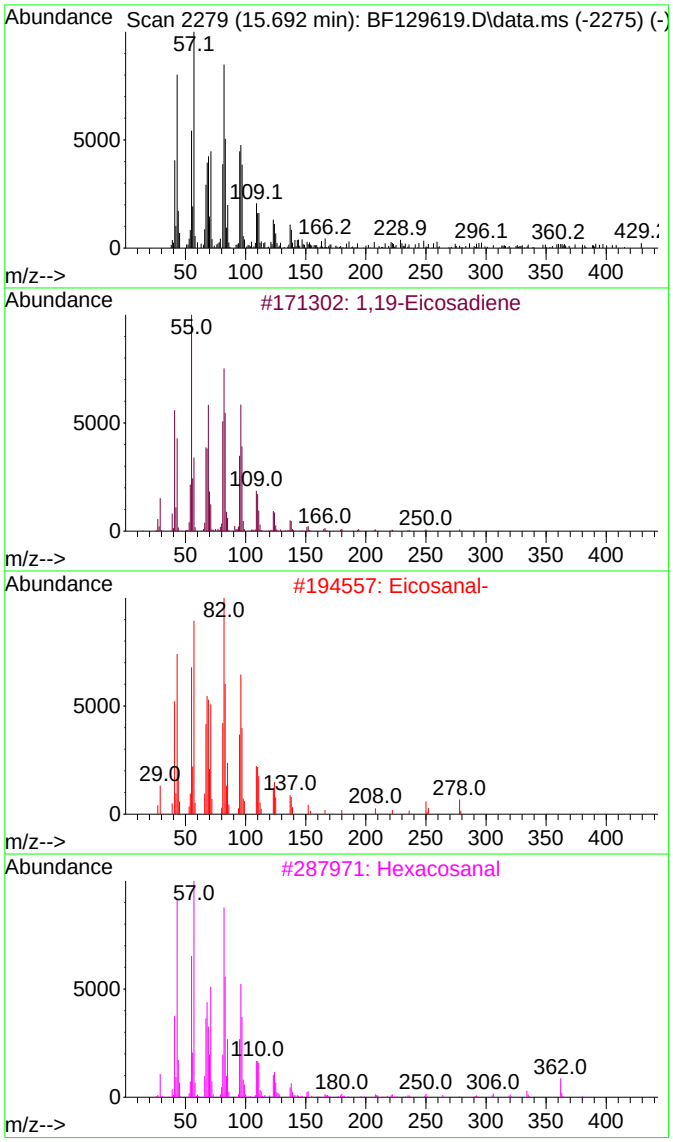
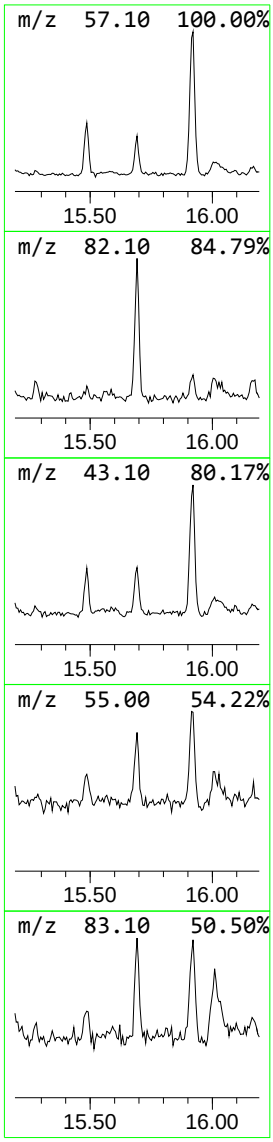
Peak Number 10 Eicosanal- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.692	4.63 ng	190845	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	93
2	Eicosanal-	296	C20H40O	002400-66-0	93
3	Hexacosanal	380	C26H52O	026627-85-0	93
4	Docosanal	324	C22H44O	057402-36-5	93
5	11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	92





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Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
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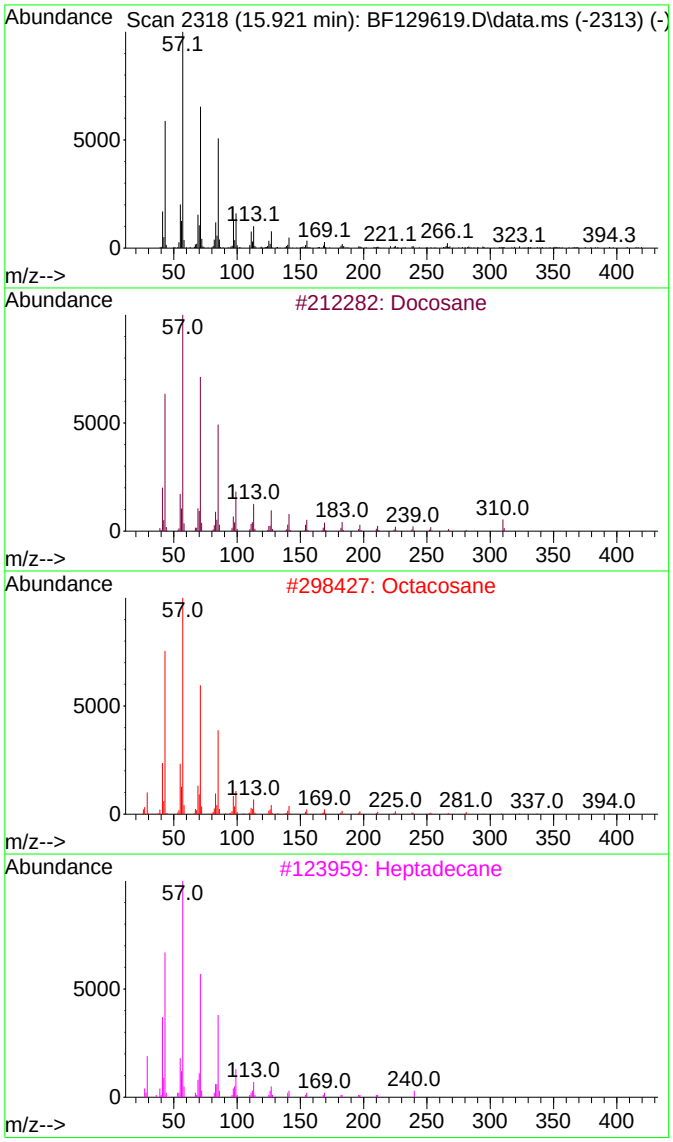
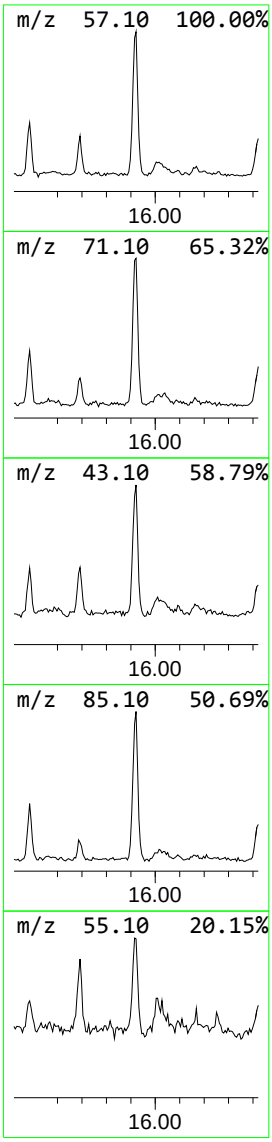
Peak Number 11 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	9.50 ng	391020	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	96
2	Octacosane	394	C28H58	000630-02-4	94
3	Heptadecane	240	C17H36	000629-78-7	93
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
5	Nonadecane	268	C19H40	000629-92-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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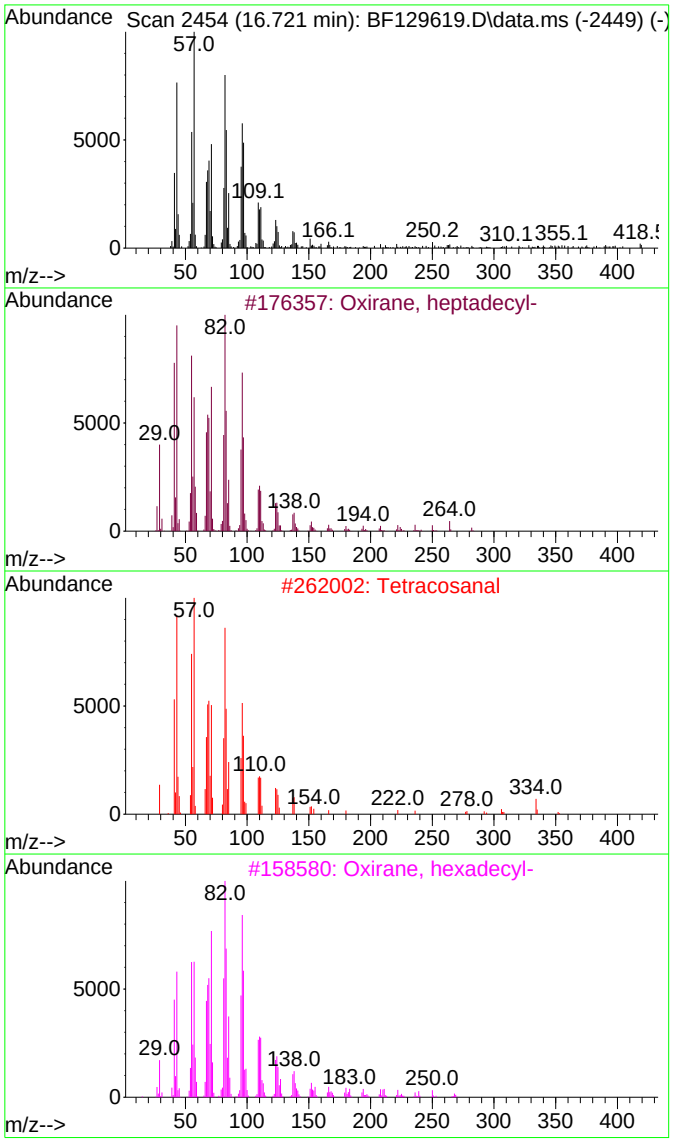
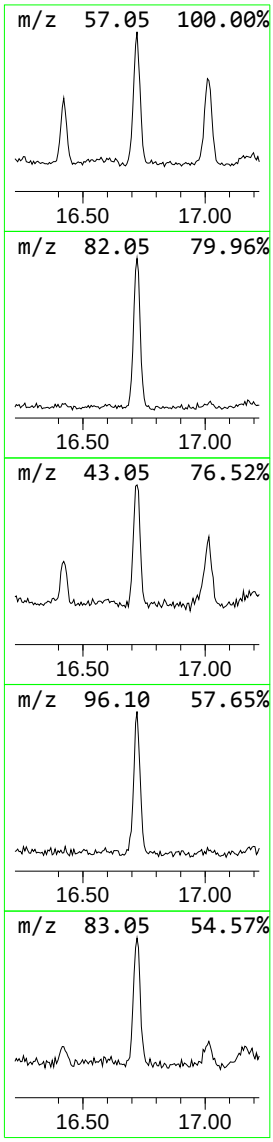
Peak Number 12 Oxirane, heptadecyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.721	11.97 ng	492990	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2	Tetracosanal	352	C24H48O	057866-08-7	93
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Heptacosanal	394	C27H54O	072934-03-3	87
5	Octacosanal	408	C28H56O	022725-64-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080522\
Data File : BF129619.D
Acq On : 06 Aug 2022 01:45
Operator : CG\JU
Sample : N3961-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-168

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
2-Pentanone, 4-...	5.075	3.8	ng	171634	1	6.845	900677	20.0
Hexadecanoic ac...	11.751	2.7	ng	140975	4	11.374	1032240	20.0
n-Hexadecanoic ...	11.892	2.2	ng	112383	4	11.374	1032240	20.0
10-Octadecenoic...	12.457	2.8	ng	143805	4	11.374	1032240	20.0
1-Docosene	13.851	8.0	ng	374848	5	14.021	936423	20.0
Triphenylphosph...	14.110	7.6	ng	353815	5	14.021	936423	20.0
Tetracosane	14.469	2.9	ng	137241	5	14.021	936423	20.0
Docosane	14.768	2.1	ng	87950	6	15.492	823577	20.0
1,19-Eicosadiene	14.916	3.2	ng	131250	6	15.492	823577	20.0
Eicosanal-	15.692	4.6	ng	190845	6	15.492	823577	20.0
Octacosane	15.921	9.5	ng	391020	6	15.492	823577	20.0
Oxirane, heptad...	16.721	12.0	ng	492990	6	15.492	823577	20.0