LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126088.D
Acq On : 9 Nov 2021 18:44
Operator : JU/CG
Sample : M4574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B6-110521-0-10

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	14	24	rVB	1722269	2215560	35.71%	5.309%
2	5.475	570	576	579	rBV	5156746	4842111	78.03%	11.603%
3	6.481	741	747	750	rBV	4896698	5084524	81.94%	12.184%
4	6.851	806	810	813	rBV	1436251	1116917	18.00%	2.676%
5	7.416	900	906	908	rBV	3275722	3409188	54.94%	8.169%
6	8.034	1007	1011	1023	rBV	978183	975738	15.72%	2.338%
7	8.134	1023	1028	1031	rBV	1721777	1424695	22.96%	3.414%
8	9.210	1205	1211	1214	rBV	7306189	6205115	100.00%	14.869%
9	9.886	1322	1326	1329	rBV	2117388	1703727	27.46%	4.083%
10	10.675	1455	1460	1463	rBV	4873449	4172783	67.25%	9.999%
11	11.369	1574	1578	1584	rBV	2152909	1758919	28.35%	4.215%
12	11.433	1584	1589	1593	rVB2	174500	206959	3.34%	0.496%
13	11.763	1644	1645	1649	rVB	93289	72326	1.17%	0.173%
14	12.580	1778	1784	1787	rBV	54652	70631	1.14%	0.169%
15	12.957	1843	1848	1851	rBV	6302234	5187575	83.60%	12.431%
16	13.857	1997	2001	2012	rBV	331541	450316	7.26%	1.079%
17	14.004	2022	2026	2030	rBV	1105243	1029746	16.60%	2.468%
18	14.768	2152	2156	2169	rBV2	167033	243140	3.92%	0.583%
19	14.974	2187	2191	2200	rVV8	118877	204923	3.30%	0.491%
20	15.074	2204	2208	2211	rVB6	78228	128165	2.07%	0.307%
21	15.468	2270	2275	2280	rBV	825838	1002784	16.16%	2.403%
22	16.451	2438	2442	2451	rVB4	69917	129821	2.09%	0.311%
23	17.045	2539	2543	2550	rVB4	50637	96371	1.55%	0.231%

Sum of corrected areas: 41732034

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Instrument :
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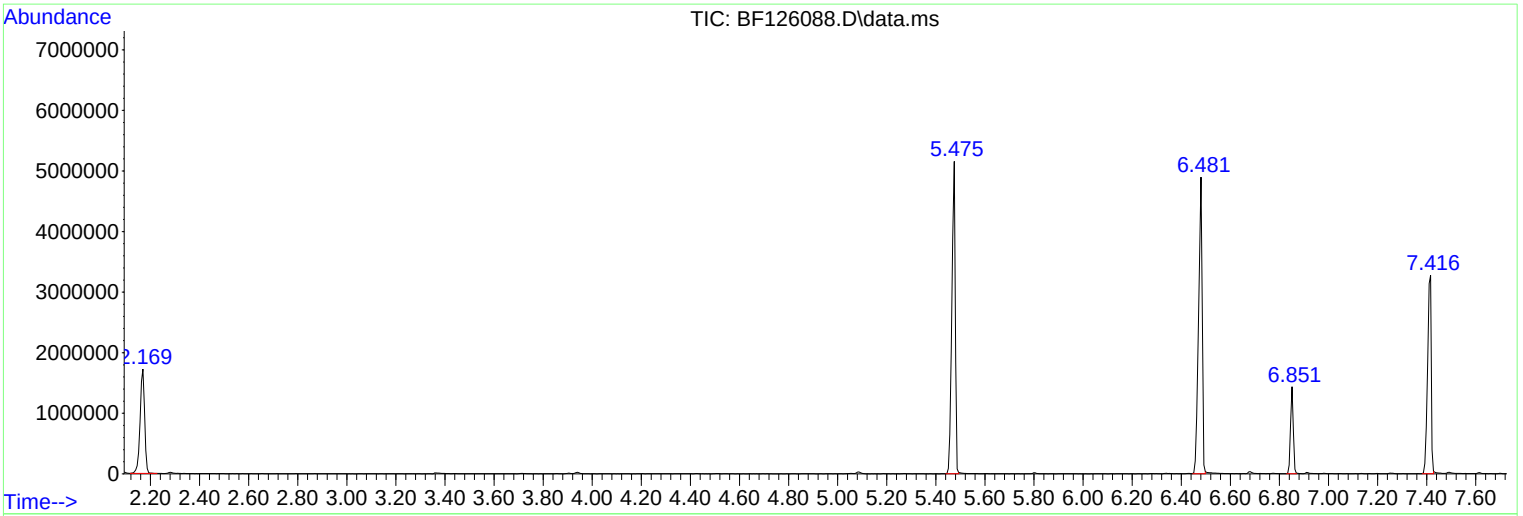
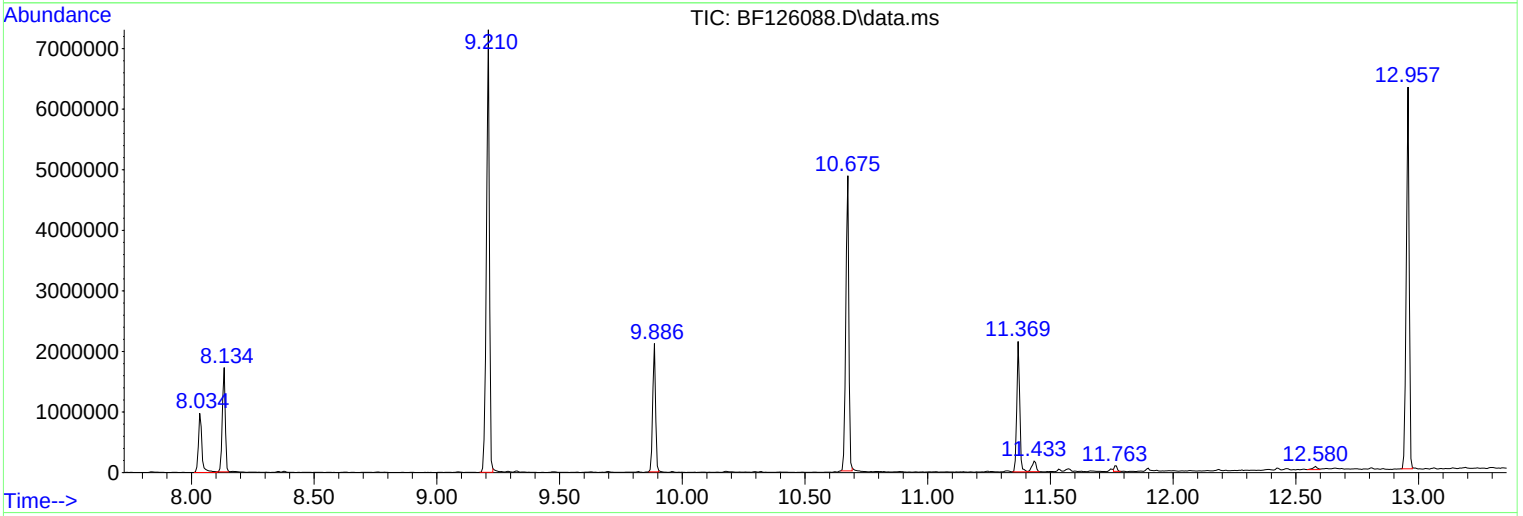
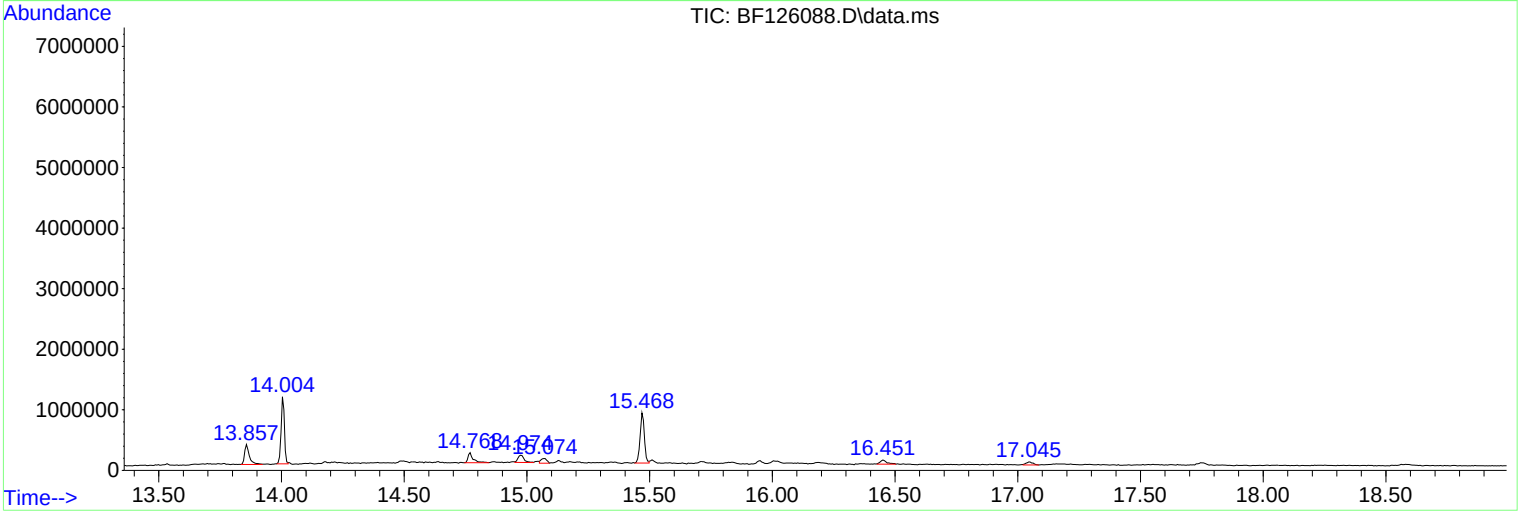
ClientSampleId :
VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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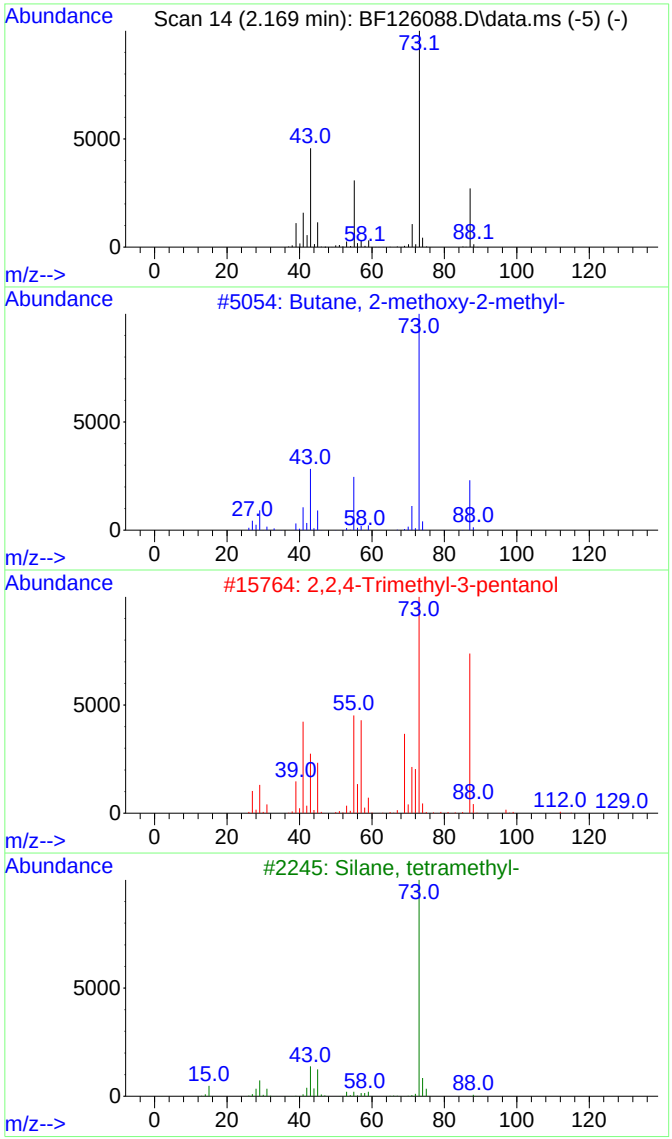
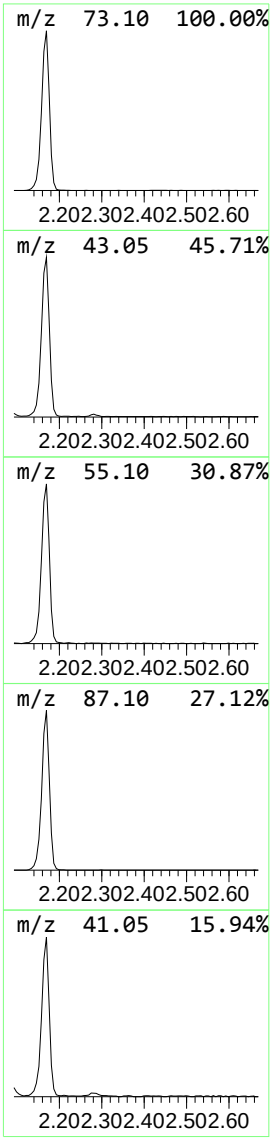
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	39.67 ng	2215560	1,4-Dichlorobenzene-d4	6.851

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF126088.D
Acq On : 9 Nov 2021 18:44
Operator : JU/CG
Sample : M4574-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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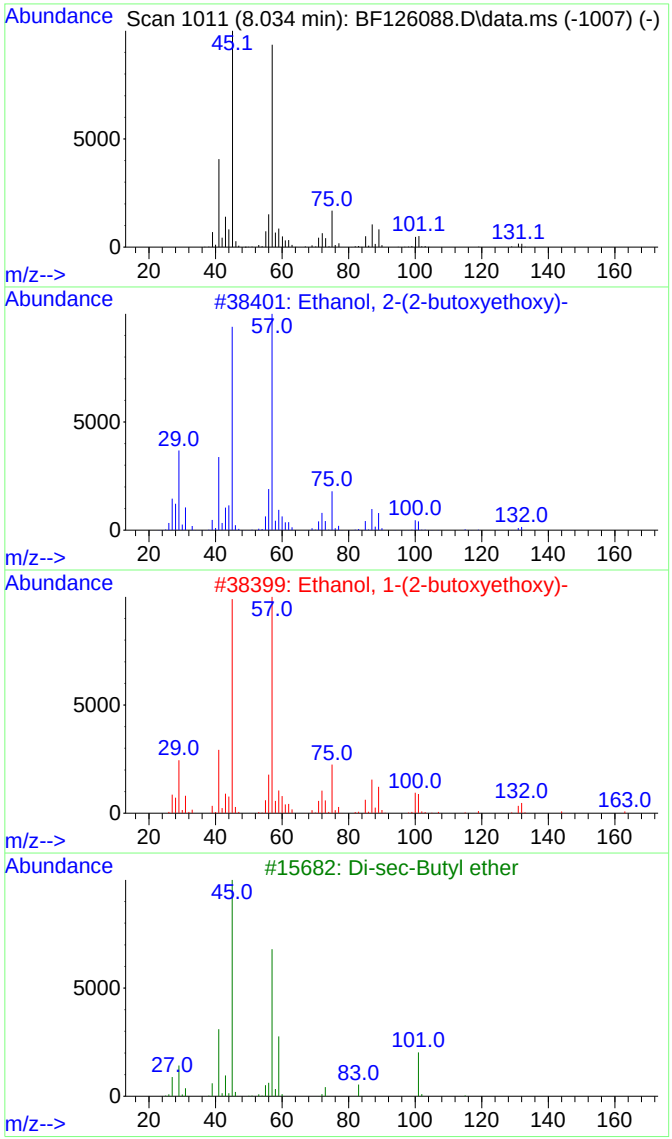
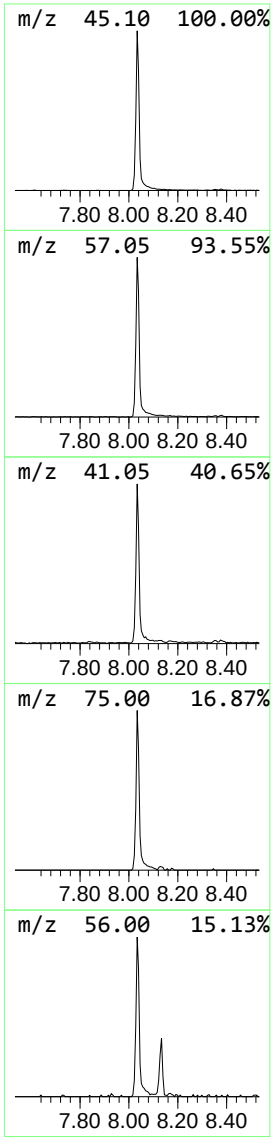
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	13.70 ng	975738	Naphthalene-d8	8.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





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Operator : JU/CG
Sample : M4574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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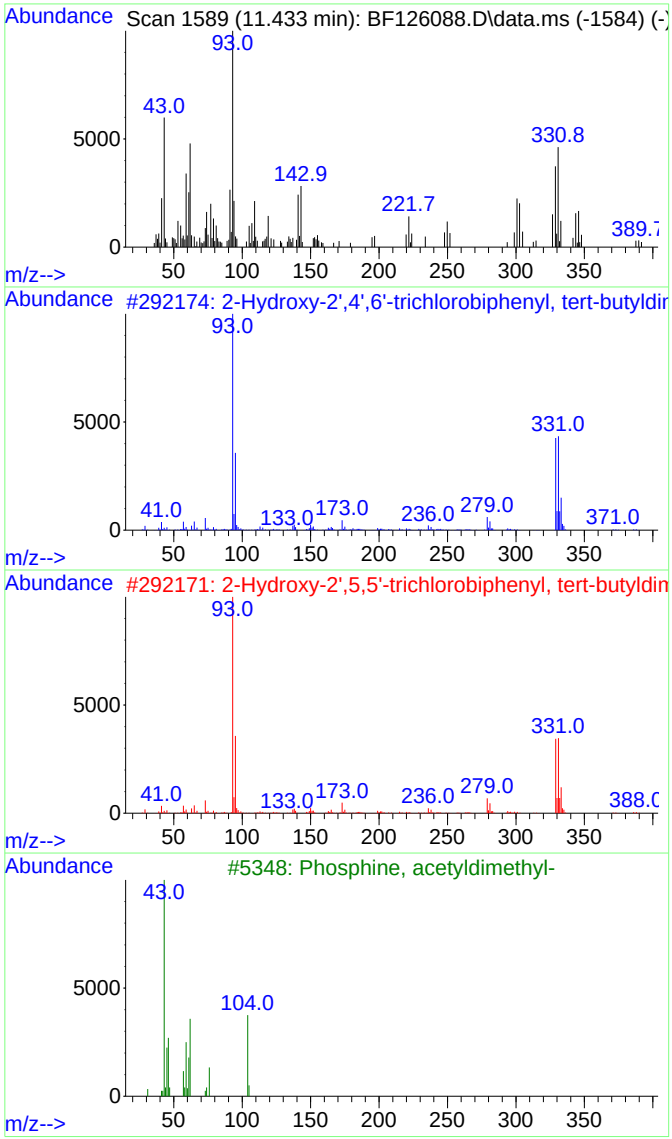
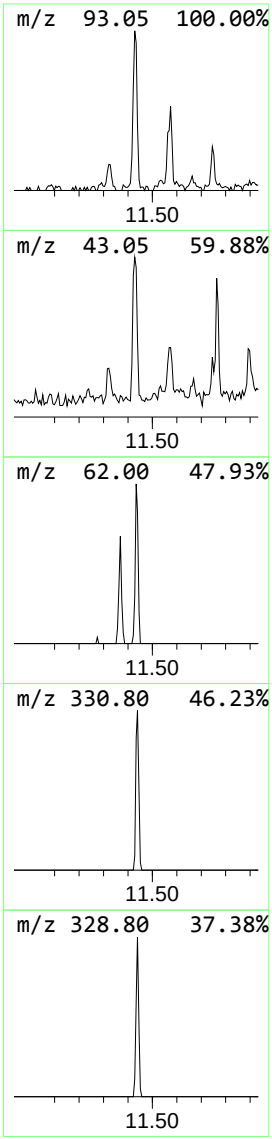
****

Peak Number 3 unknown11.433 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.433	2.35 ng	206959	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-2',4',6'-trichlorobiph...	386	C18H21Cl3OSi	1000447-67-1	27
2	2-Hydroxy-2',5,5'-trichlorobiphe...	386	C18H21Cl3OSi	1000447-67-9	16
3	Phosphine, acetyldimethyl-	104	C4H9OP	018983-86-3	12
4	2-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-67-3	10
5	Propanoic acid, 2-chloro-, ethyl...	136	C5H9ClO2	000535-13-7	9





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Data File : BF126088.D
Acq On : 9 Nov 2021 18:44
Operator : JU/CG
Sample : M4574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

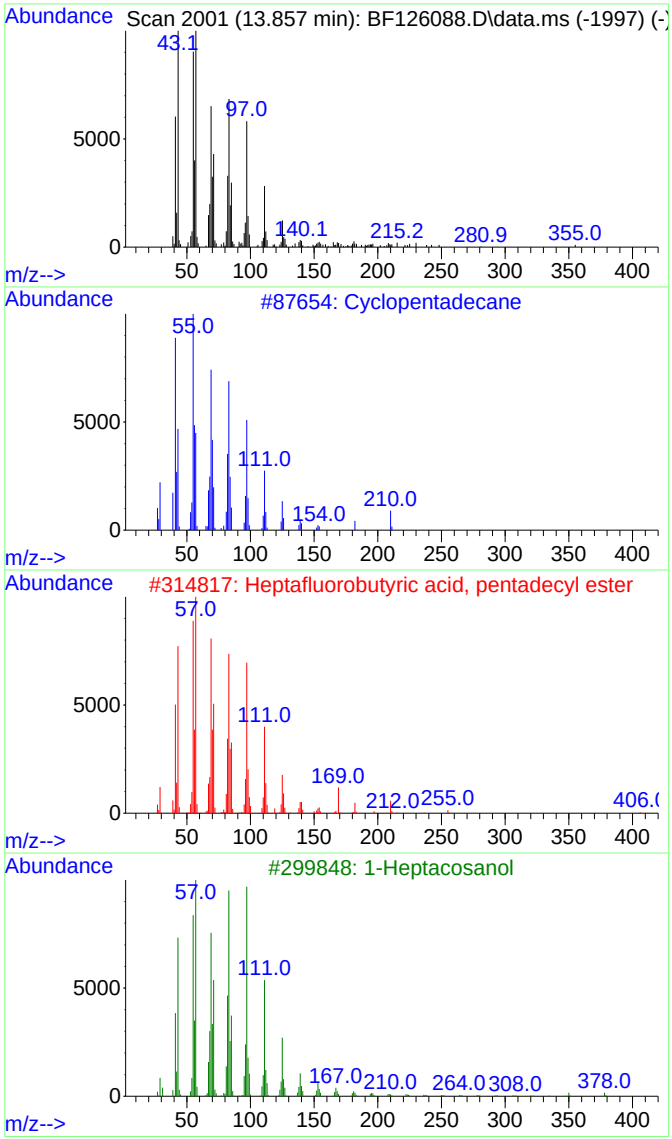
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

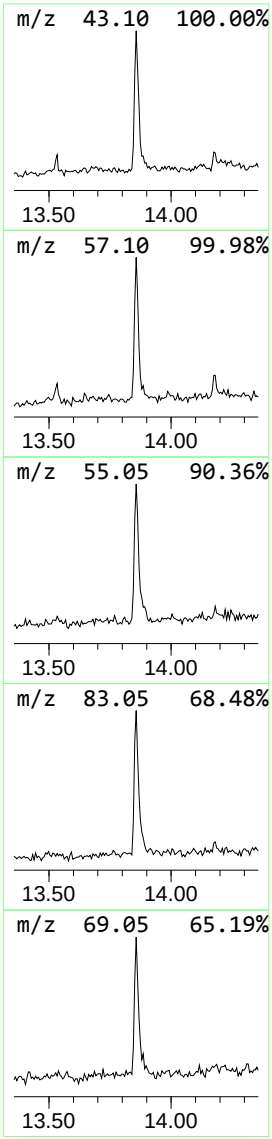
****

Peak Number 4 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	8.75 ng	450316	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





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Sample : M4574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

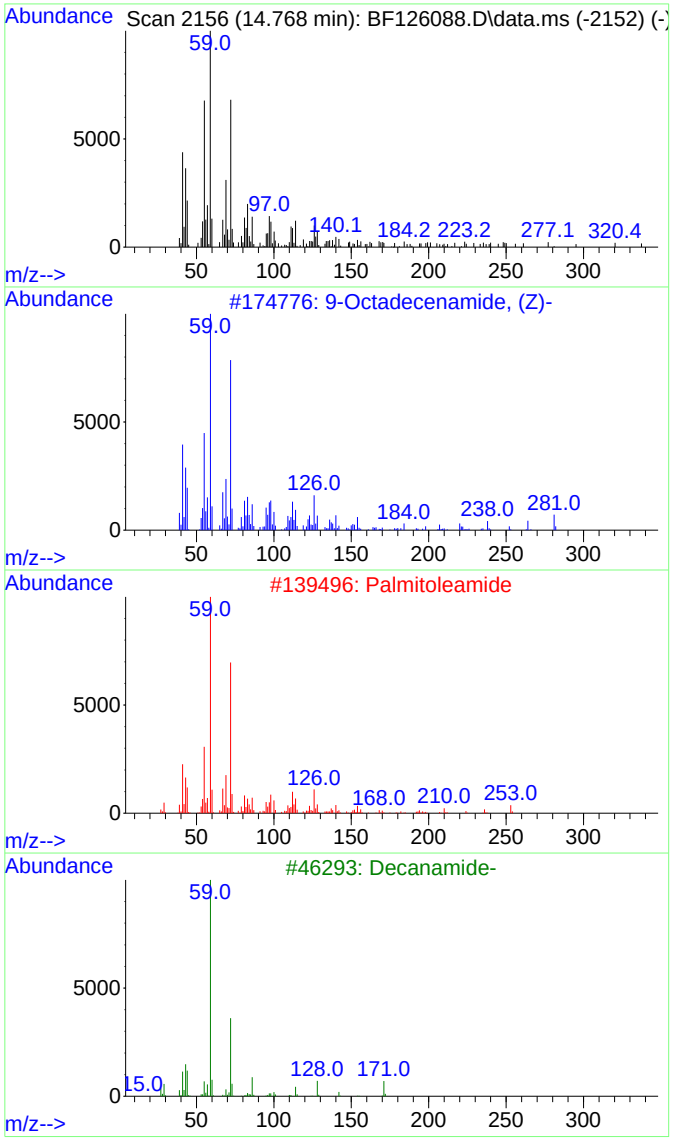
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

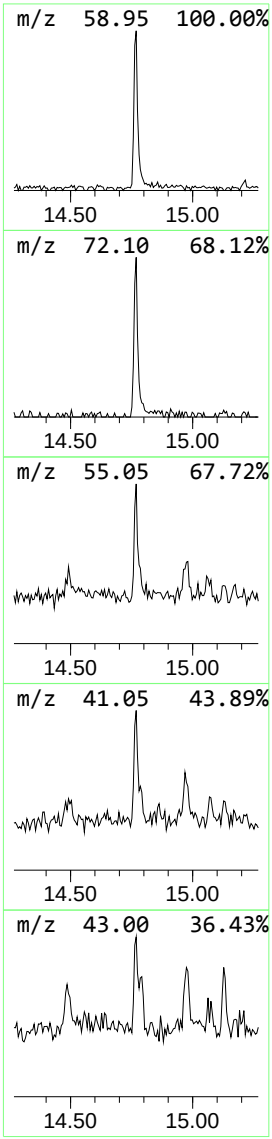
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	4.85 ng	243140	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Palmitoleamide	253	C16H31NO	106010-22-4	64
3	Decanamide-	171	C10H21NO	002319-29-1	58
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	58
5	Hexanamide	115	C6H13NO	000628-02-4	35





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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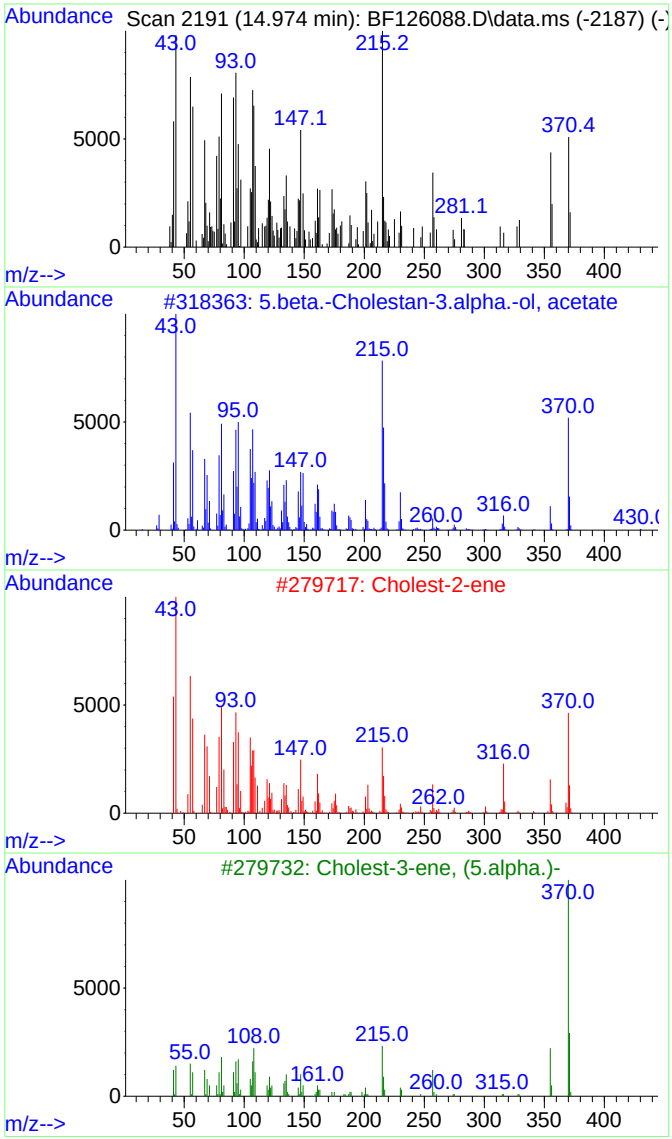
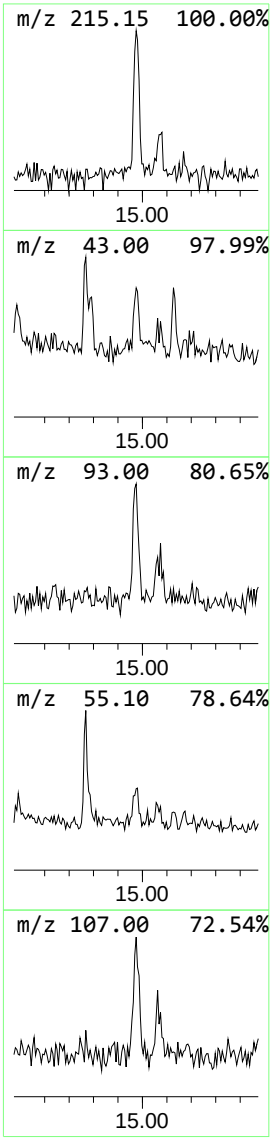
****
Peak Number 6 5.beta.-Cholestan-3.alpha.-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	4.09 ng	204923	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.beta.-Cholestan-3.alpha.-ol, a...	430	C29H50O2	033157-47-0	52
2	Cholest-2-ene	370	C27H46	015910-23-3	45
3	Cholest-3-ene, (5.alpha.)-	370	C27H46	028338-69-4	45
4	17-(1,5-Dimethylhexyl)-10,13-dim...	370	C27H46	1000210-50-1	42
5	5,8,11,14,17-Eicosapentaenoic ac...	316	C21H32O2	002734-47-6	38





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VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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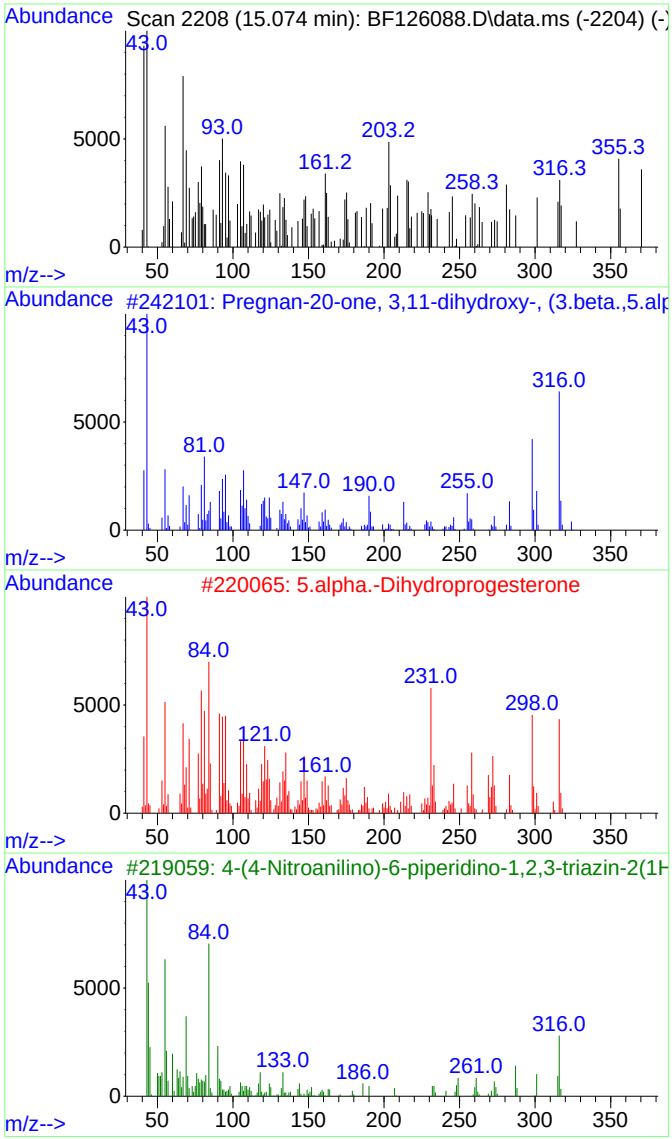
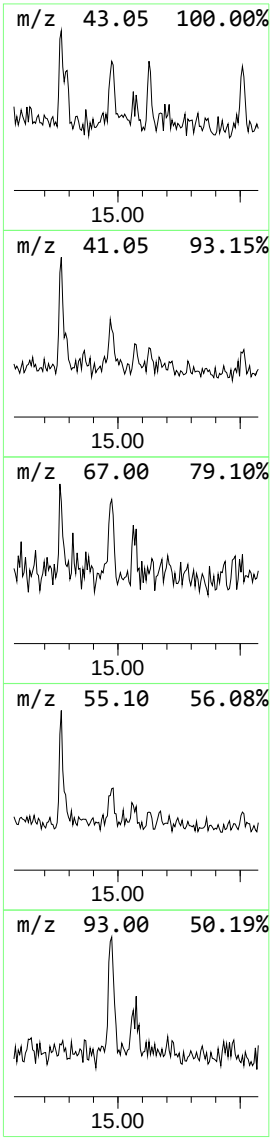
****

Peak Number 7 unknown15.074 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	2.56 ng	128165	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pregnan-20-one, 3,11-dihydroxy-,...	334	C21H34O3	000565-91-3	10
2	5.alpha.-Dihydroprogesterone	316	C21H32O2	000566-65-4	10
3	4-(4-Nitroanilino)-6-piperidino-...	316	C14H16N6O3	320367-58-6	10
4	4-n-Butyl-3-[n-octylsulfonyl]nit...	355	C18H29NO4S	1000214-51-2	9
5	3.beta.-Acetoxy-16-isothiocyanat...	415	C24H33NO3S	006084-08-8	9





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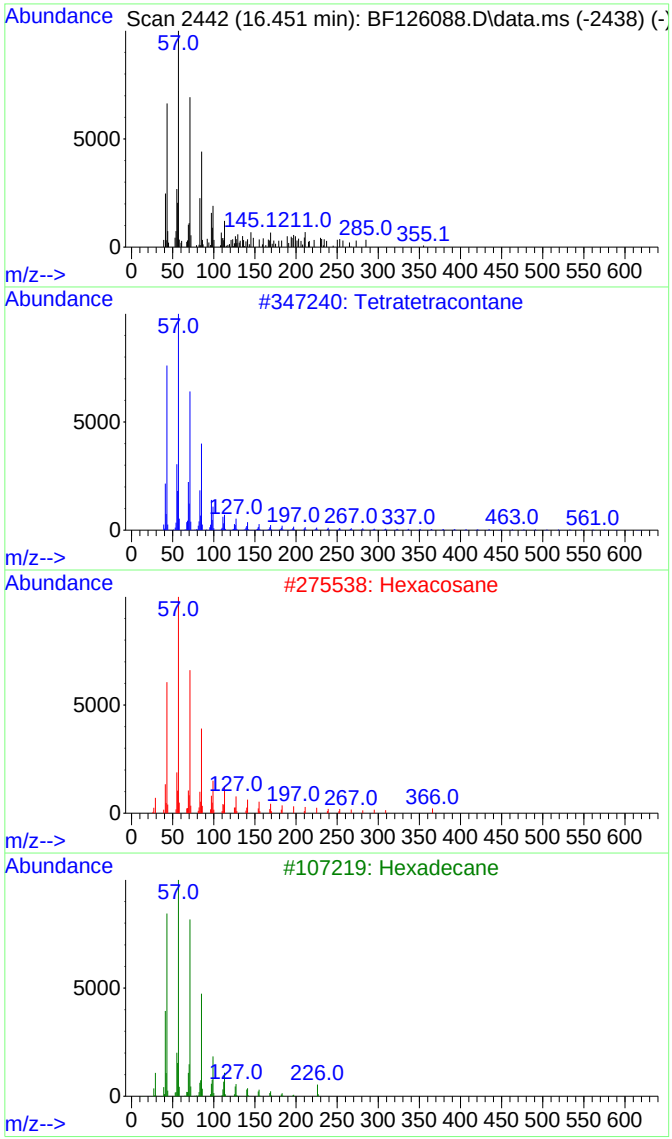
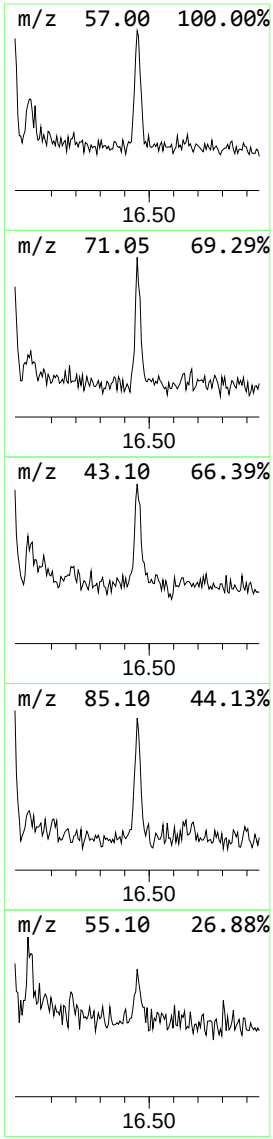
****

Peak Number 8 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.451	2.59 ng	129821	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	64
2	Hexacosane	366	C26H54	000630-01-3	64
3	Hexadecane	226	C16H34	000544-76-3	58
4	6,6-Diethylhexadecane	282	C20H42	1000360-41-4	53
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	53





Tentatively Identified Compound (LSC) summary

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Data File : BF126088.D
Acq On : 9 Nov 2021 18:44
Operator : JU/CG
Sample : M4574-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VWE-B6-110521-0-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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...	2.169	39.7	ng	2215560	1	6.851	1116920	20.0
Ethanol, 2-(2-b...	8.034	13.7	ng	975738	2	8.134	1424700	20.0
unknown11.433	11.433	2.4	ng	206959	4	11.369	1758920	20.0
Cyclopentadecane	13.857	8.8	ng	450316	5	14.004	1029750	20.0
9-Octadecenamid...	14.768	4.8	ng	243140	6	15.468	1002780	20.0
5.beta.-Cholest...	14.974	4.1	ng	204923	6	15.468	1002780	20.0
unknown15.074	15.074	2.6	ng	128165	6	15.468	1002780	20.0
Tetratetracontane	16.451	2.6	ng	129821	6	15.468	1002780	20.0