LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128661.D
Acq On : 03 Jun 2022 02:38
Operator : CG\JU
Sample : N2989-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS008-0006-01

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	463	467	472	rVB	78972	91206	4.52%	0.636%
2	5.475	538	542	554	rBV	1461997	1617051	80.19%	11.280%
3	6.486	711	714	725	rBV	1617233	1622928	80.48%	11.321%
4	6.822	767	771	774	rBV	696791	521255	25.85%	3.636%
5	7.386	862	867	870	rBV	1253825	1135088	56.29%	7.918%
6	8.104	985	989	993	rBV	803282	639554	31.72%	4.461%
7	9.180	1168	1172	1176	rBV	2256721	2016504	100.00%	14.067%
8	9.863	1284	1288	1291	rBV	850063	696120	34.52%	4.856%
9	10.651	1418	1422	1426	rBV	1355315	1166354	57.84%	8.136%
10	11.351	1537	1541	1544	rBV	787264	668680	33.16%	4.665%
11	11.880	1628	1631	1634	rBV	130609	111594	5.53%	0.778%
12	11.916	1634	1637	1640	rVB	113710	97226	4.82%	0.678%
13	12.668	1761	1765	1772	rBV2	96991	101865	5.05%	0.711%
14	12.939	1807	1811	1814	rBV	1954202	1604537	79.57%	11.193%
15	13.798	1954	1957	1962	rVB	46066	45708	2.27%	0.319%
16	13.910	1969	1976	1984	rBV7	38777	133114	6.60%	0.929%
17	13.992	1984	1990	1993	rVB2	584588	616379	30.57%	4.300%
18	14.086	2001	2006	2010	rBV	171855	197335	9.79%	1.377%
19	14.127	2010	2013	2016	rVV	68013	67100	3.33%	0.468%
20	14.168	2016	2020	2022	rVV2	105170	97002	4.81%	0.677%
21	14.198	2022	2025	2027	rVV2	38112	38177	1.89%	0.266%
22	14.221	2027	2029	2032	rVB	41243	32949	1.63%	0.230%
23	14.374	2050	2055	2056	rBV3	19177	24860	1.23%	0.173%
24	14.468	2068	2071	2074	rVB2	29228	29721	1.47%	0.207%
25	15.115	2178	2181	2184	rBV	28204	28916	1.43%	0.202%
26	15.457	2234	2239	2243	rBV	407459	483307	23.97%	3.372%
27	15.933	2316	2320	2324	rVB	37444	53316	2.64%	0.372%
28	16.727	2452	2455	2462	rVB5	24791	40312	2.00%	0.281%
29	17.027	2501	2506	2512	rBV3	30985	64145	3.18%	0.447%
30	17.262	2541	2546	2554	rVB7	52276	113106	5.61%	0.789%
31	18.009	2667	2673	2677	rVB9	15782	35526	1.76%	0.248%
32	18.521	2754	2760	2780	rVB9	34788	144106	7.15%	1.005%

Sum of corrected areas: 14335041

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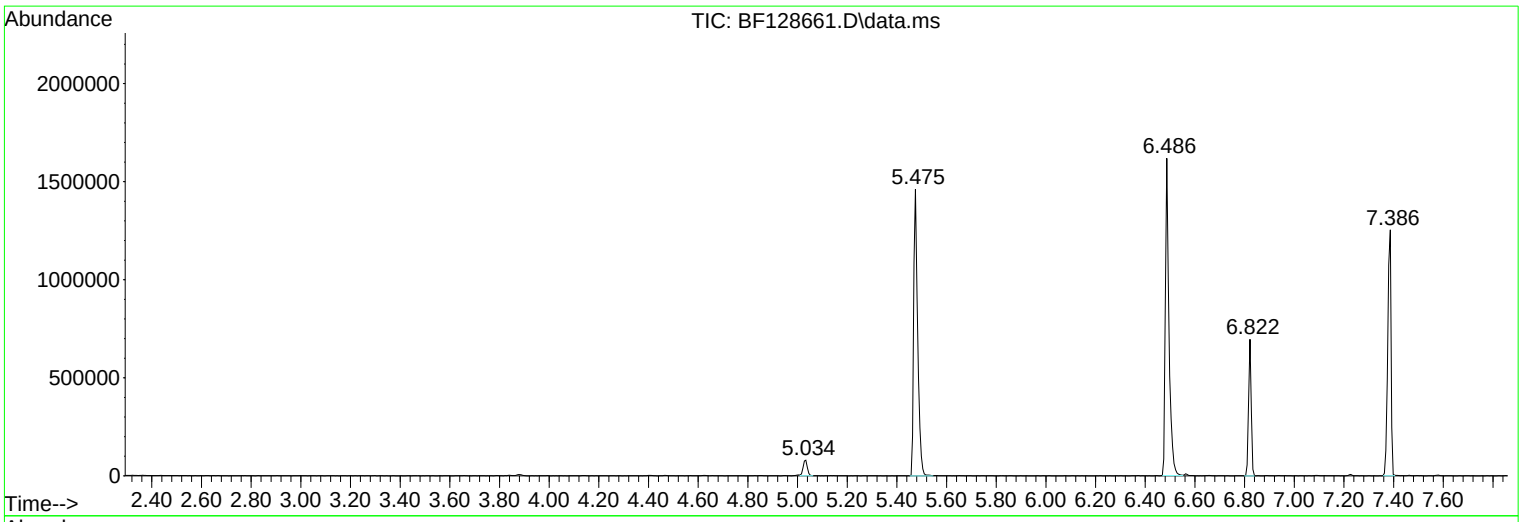
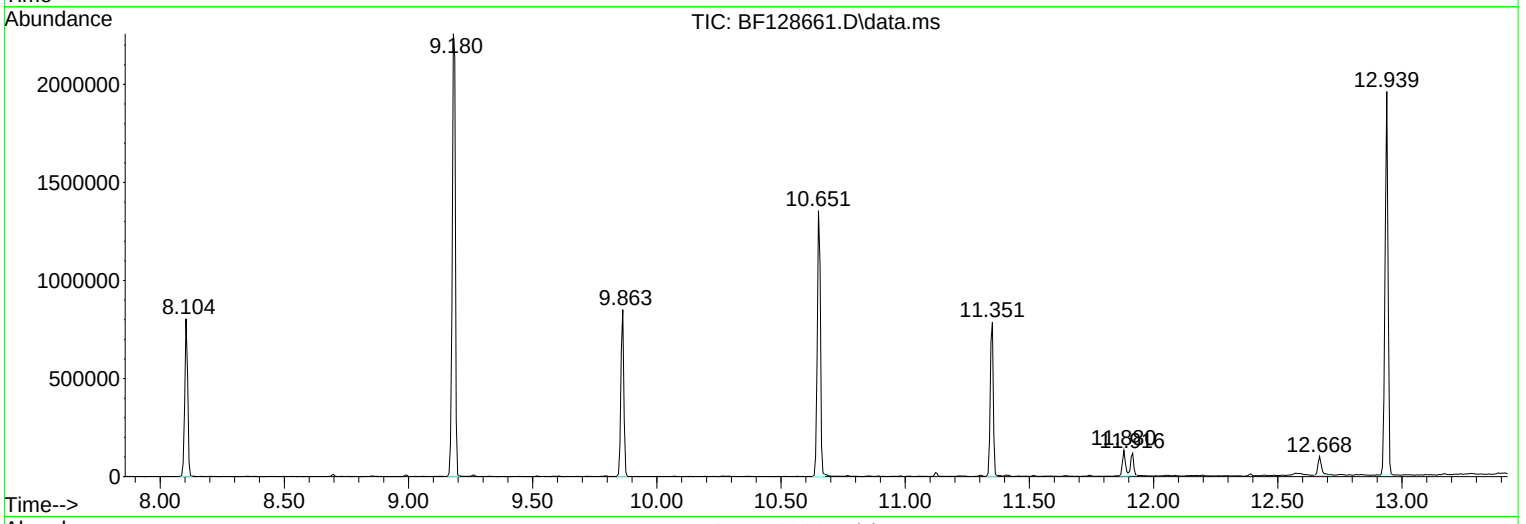
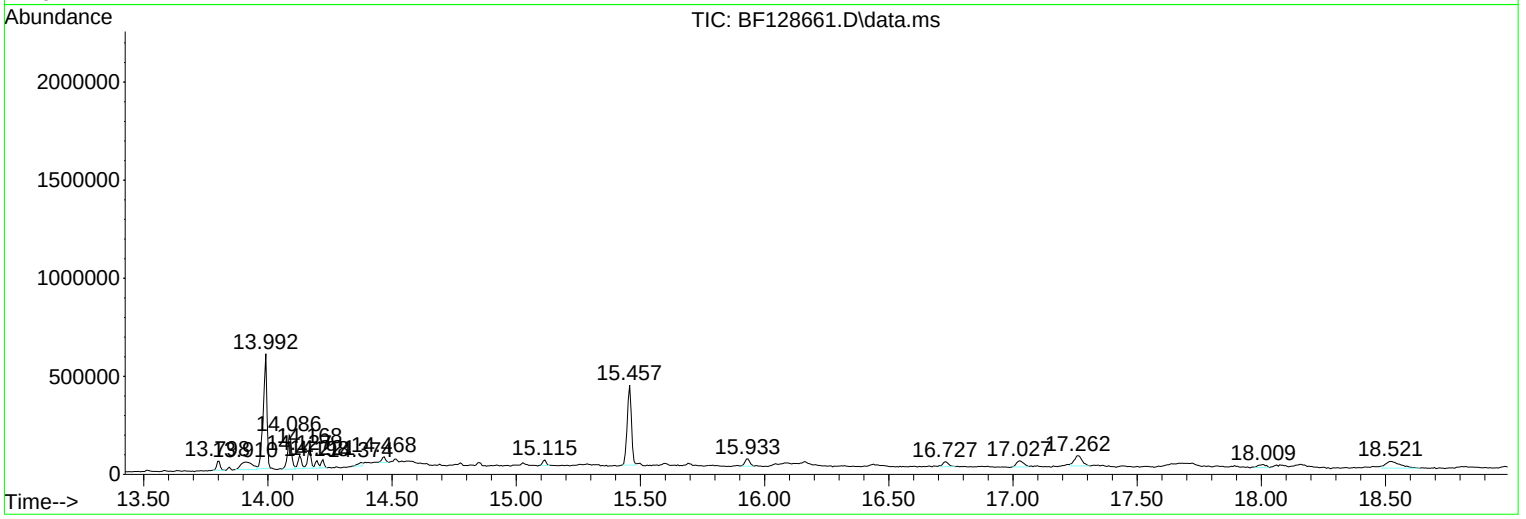
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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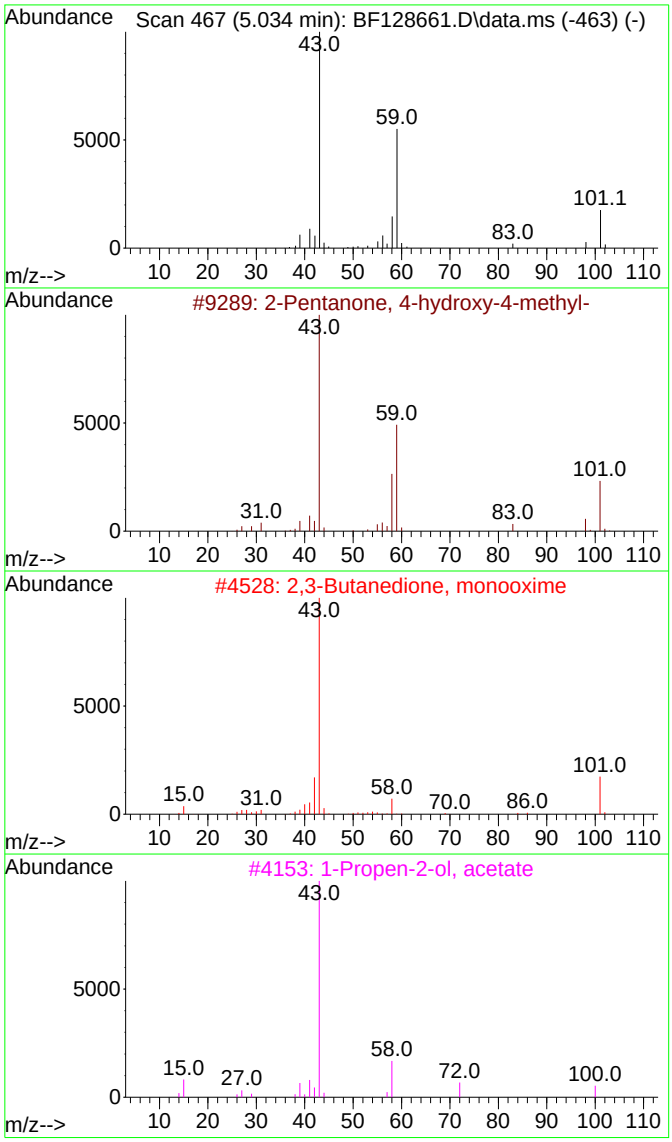
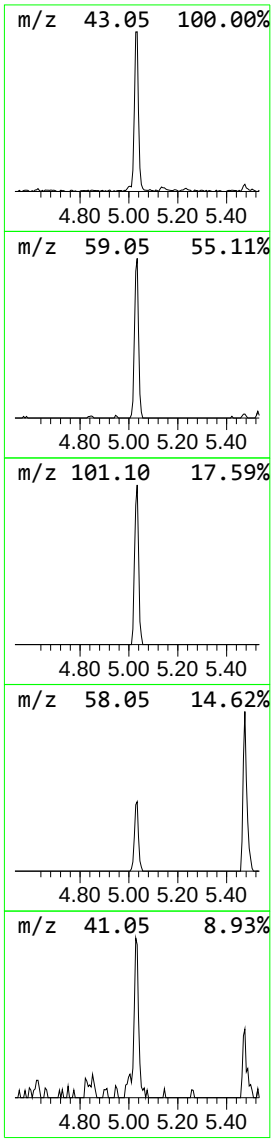
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	3.50 ng	91206	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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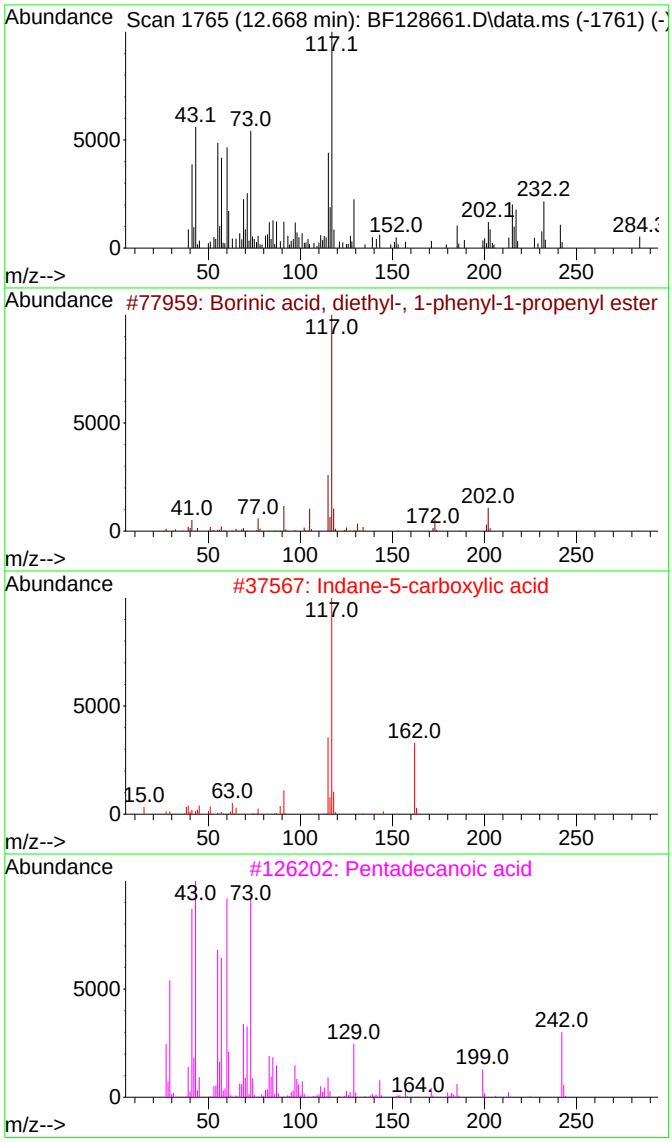
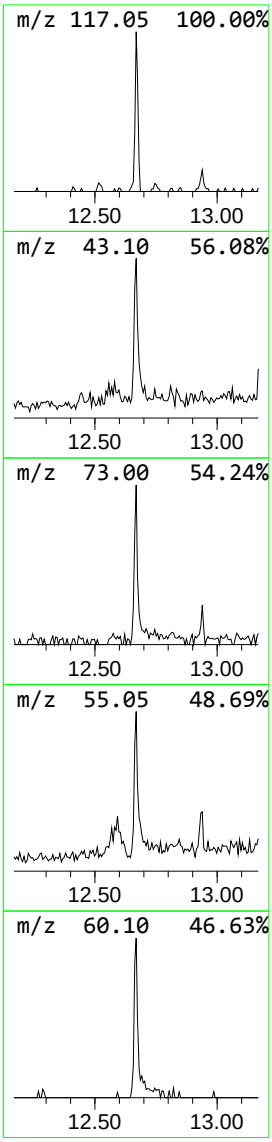
****

Peak Number 2 unknown12.668 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.668	3.05 ng	101865	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Borinic acid, diethyl-, 1-phenyl...	202	C13H19BO	034602-33-0	30
2	Indane-5-carboxylic acid	162	C10H10O2	065898-38-6	27
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	25
4	1-Methyl-1-(3-phenylprop-2-enyl)...	232	C14H20OSi	1000216-97-3	18
5	3,6-Bis(benzyl)-tetrazine	262	C16H14N4	014141-65-2	14





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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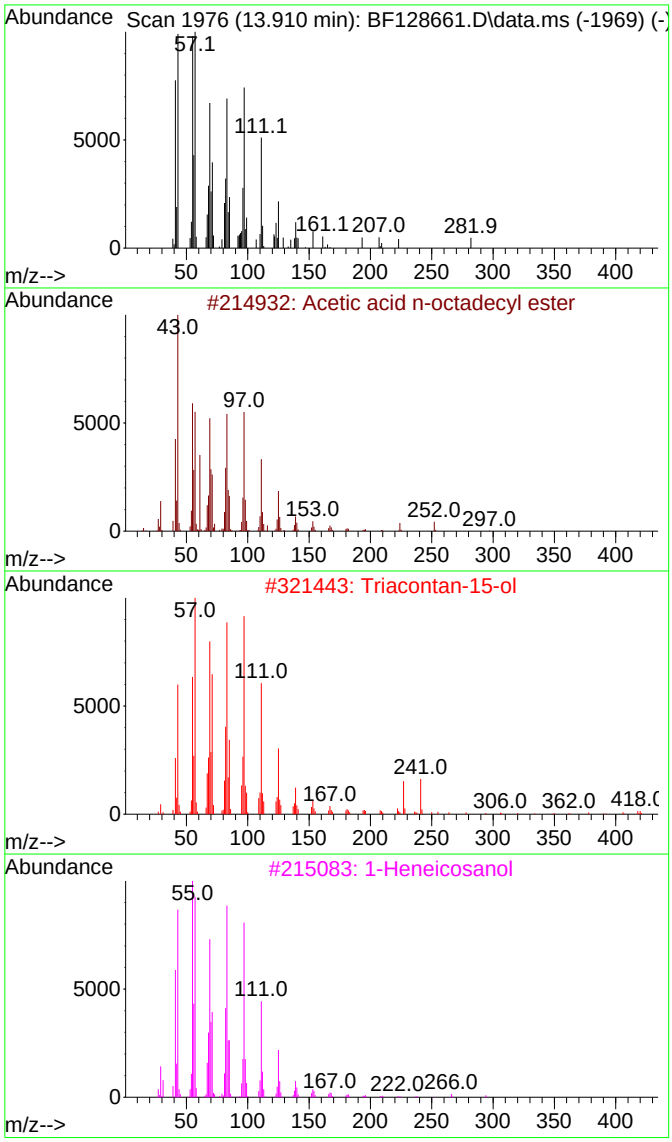
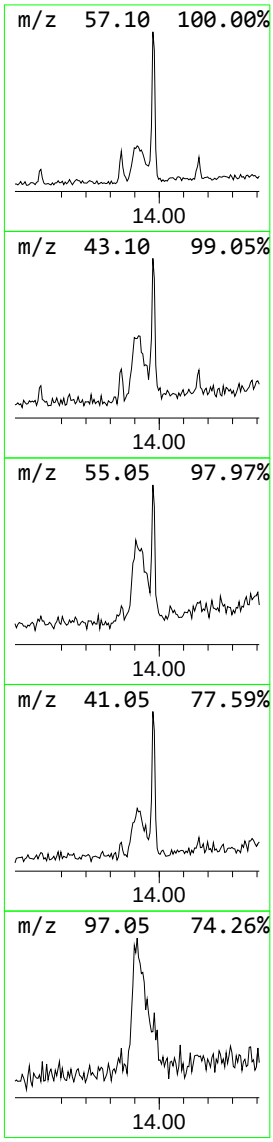
****
Peak Number 3 Acetic acid n-octadecyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	4.32 ng	133114	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	90
2	Triacontan-15-ol	438	C30H62O	031849-26-0	87
3	1-Heneicosanol	312	C21H44O	015594-90-8	83
4	Behenic alcohol	326	C22H46O	000661-19-8	83
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	80





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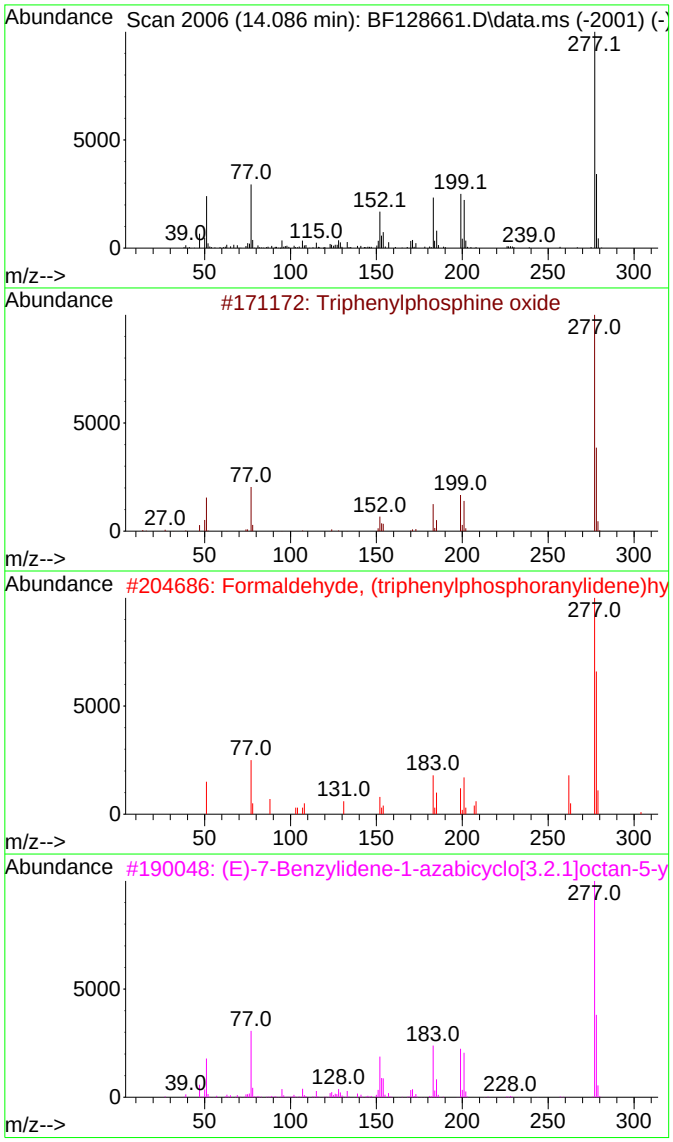
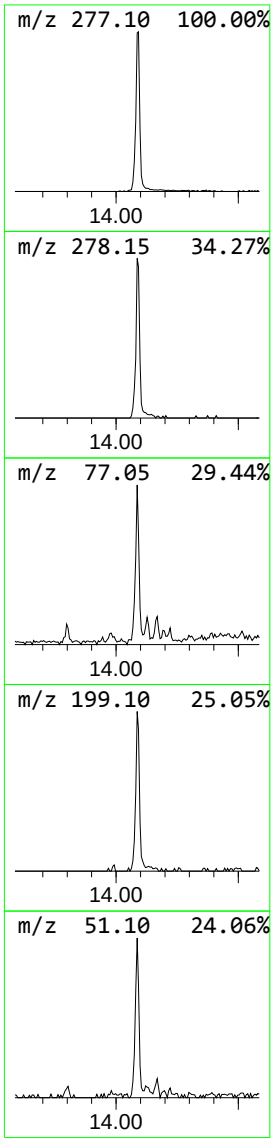
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	6.40 ng	197335	Chrysene-d12	13.992

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	64
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	53
4	Furo[3,2-c]quinoline, 8-bromo-2,...	277	C13H12BrNO	1000310-92-7	37
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35





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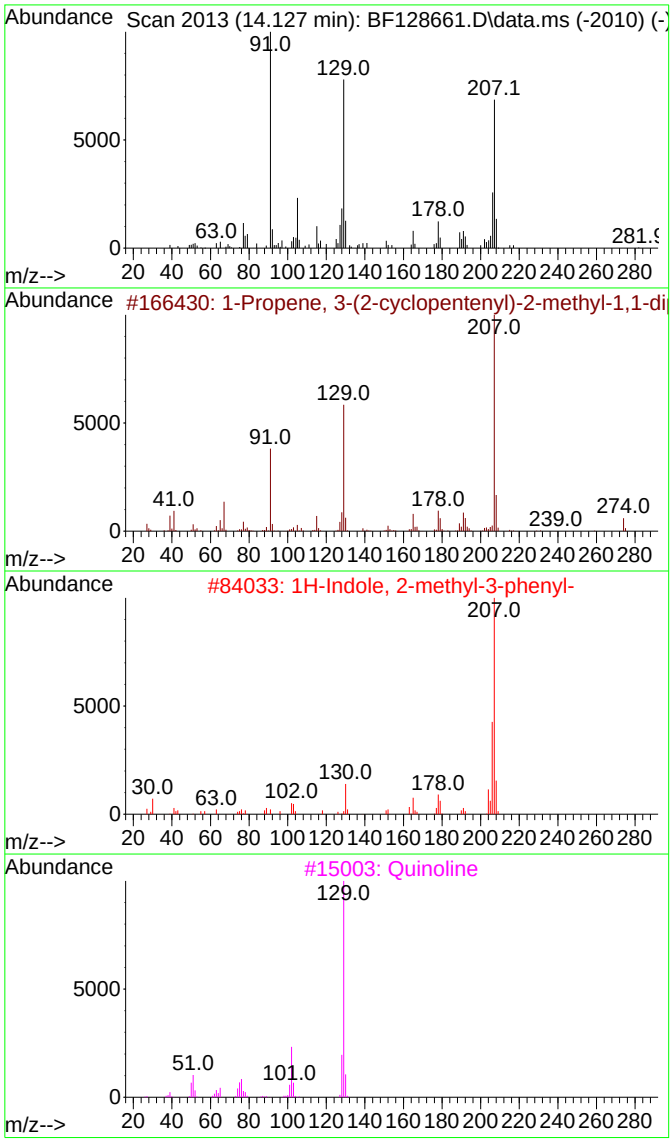
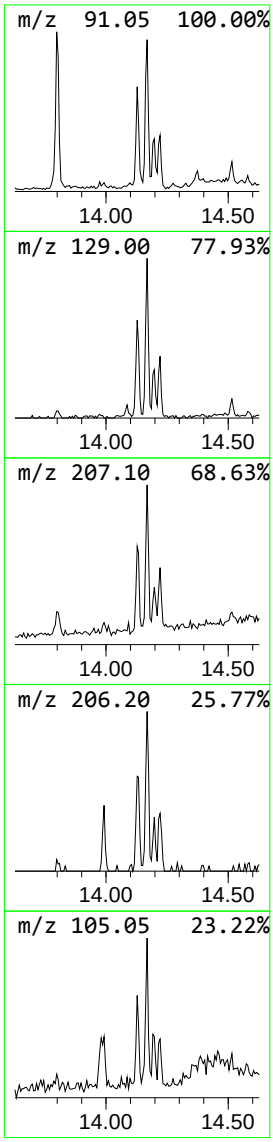
****
Peak Number 5 1-Propene, 3-(2-cyclopenten... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	2.18 ng	67100	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	64
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	42
3	Quinoline	129	C9H7N	000091-22-5	35
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	35
5	Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	35





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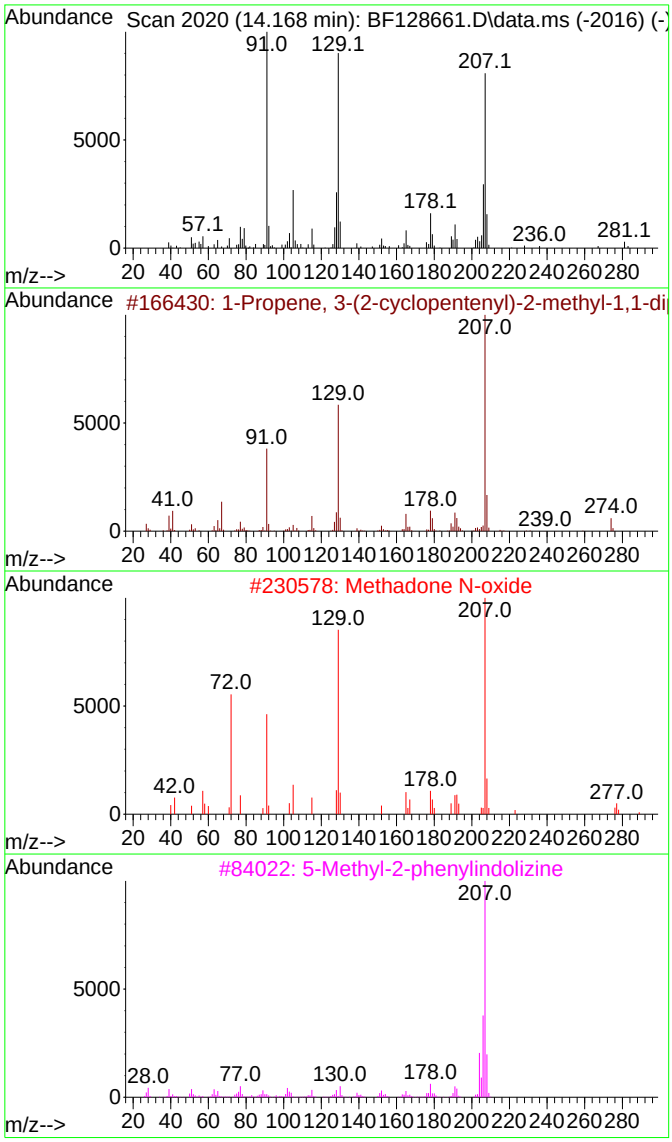
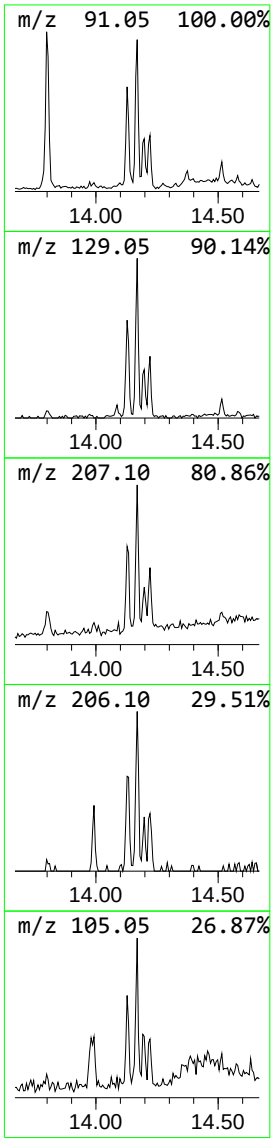
****

Peak Number 6 Methadone N-oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.168	3.15 ng	97002	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	78
2	Methadone N-oxide	325	C21H27NO2	1000120-80-7	72
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	50
4	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
5	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	45





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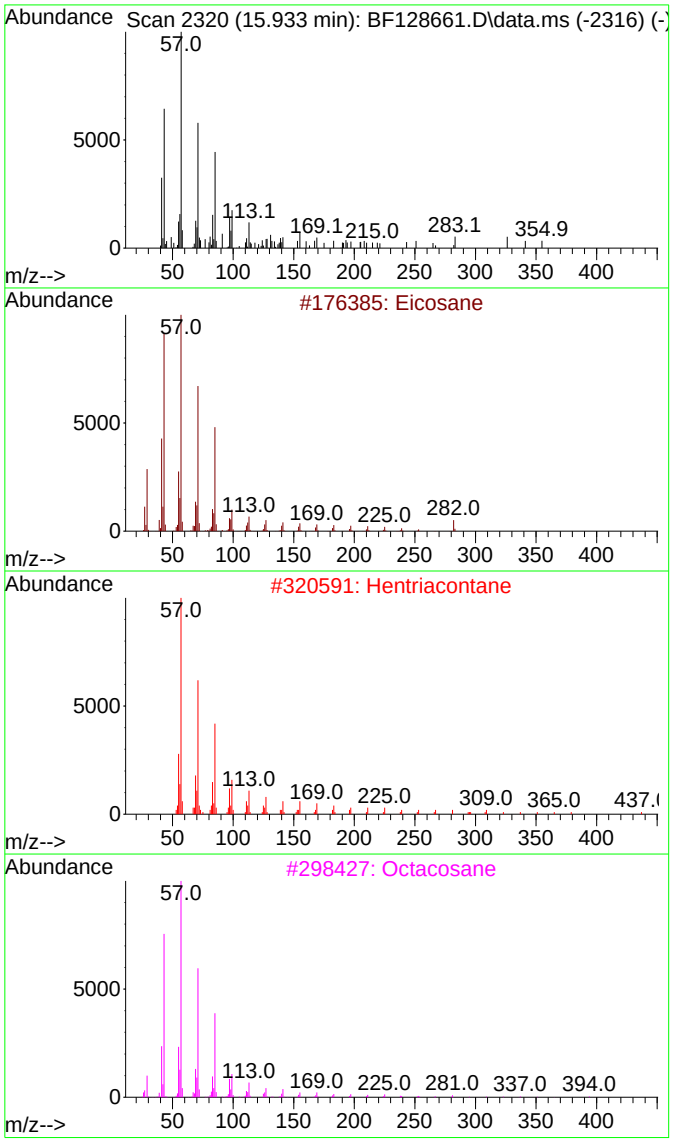
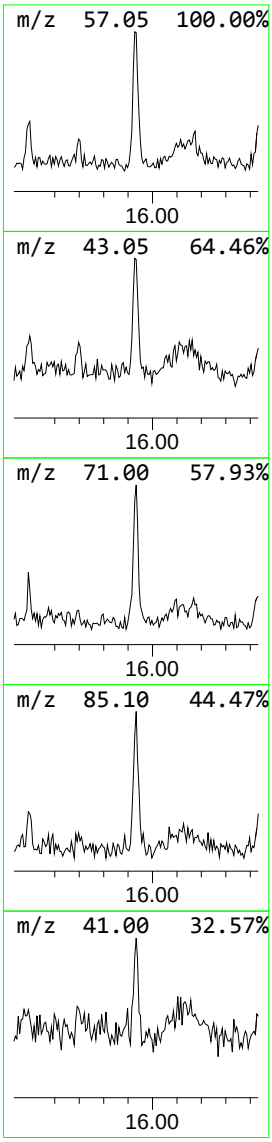
Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	2.21 ng	53316	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hentriacontane	437	C31H64	000630-04-6	86
3	Octacosane	394	C28H58	000630-02-4	83
4	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	83
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	83





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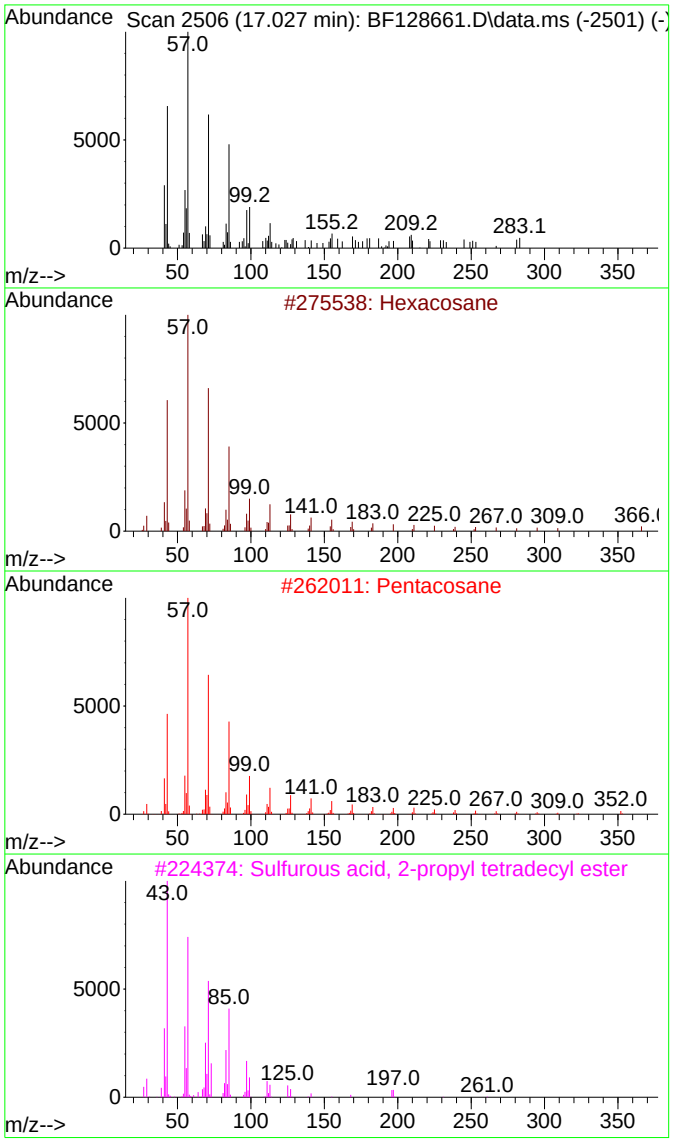
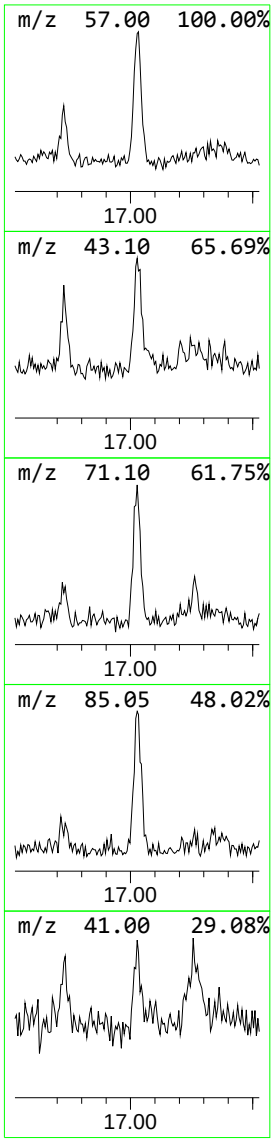
Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.027	2.65 ng	64145	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	Pentacosane	352	C25H52	000629-99-2	72
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1010309-12-5	64
4	Heneicosane	296	C21H44	000629-94-7	64
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64





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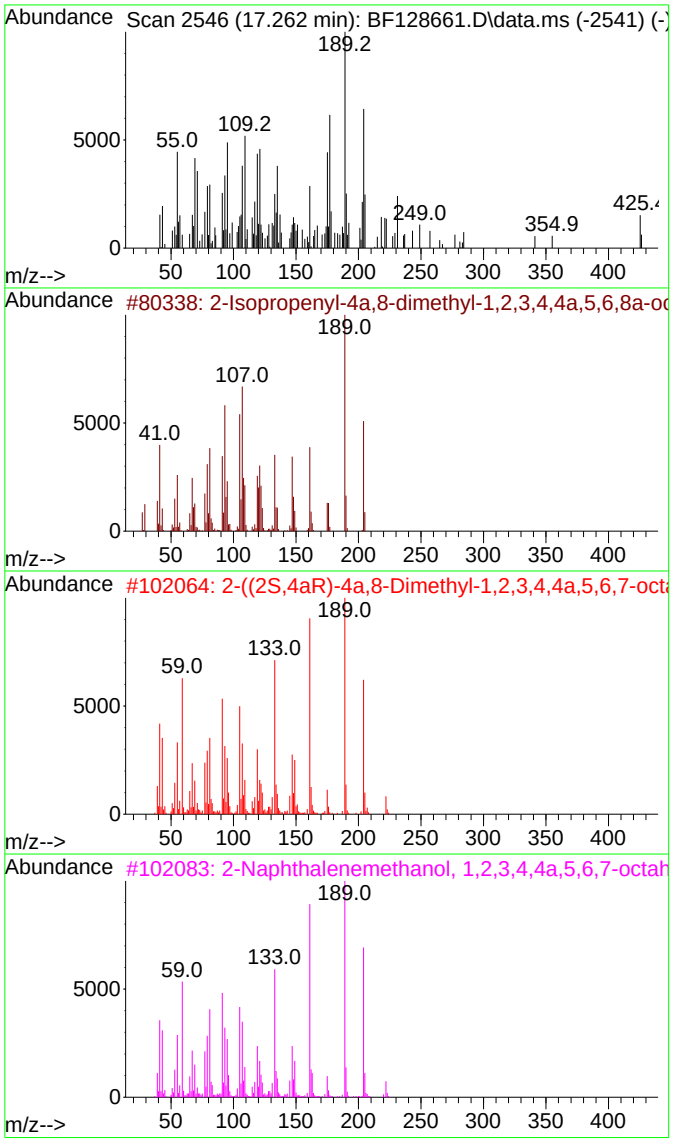
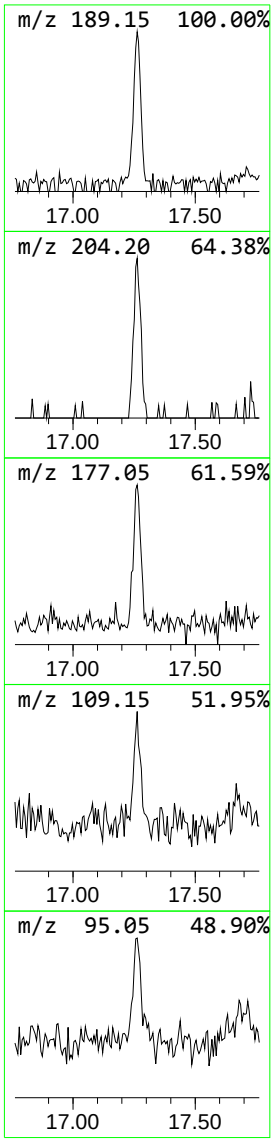
****
Peak Number 9 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	4.68 ng	113106	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	64
2	2-((2S,4aR)-4a,8-Dimethyl-1,2,3,...	222	C15H26O	117066-77-0	53
3	2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	46
4	1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	44
5	Cedrene-V6	204	C15H24	1000162-76-8	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128661.D
Acq On : 03 Jun 2022 02:38
Operator : CG\JU
Sample : N2989-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS008-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

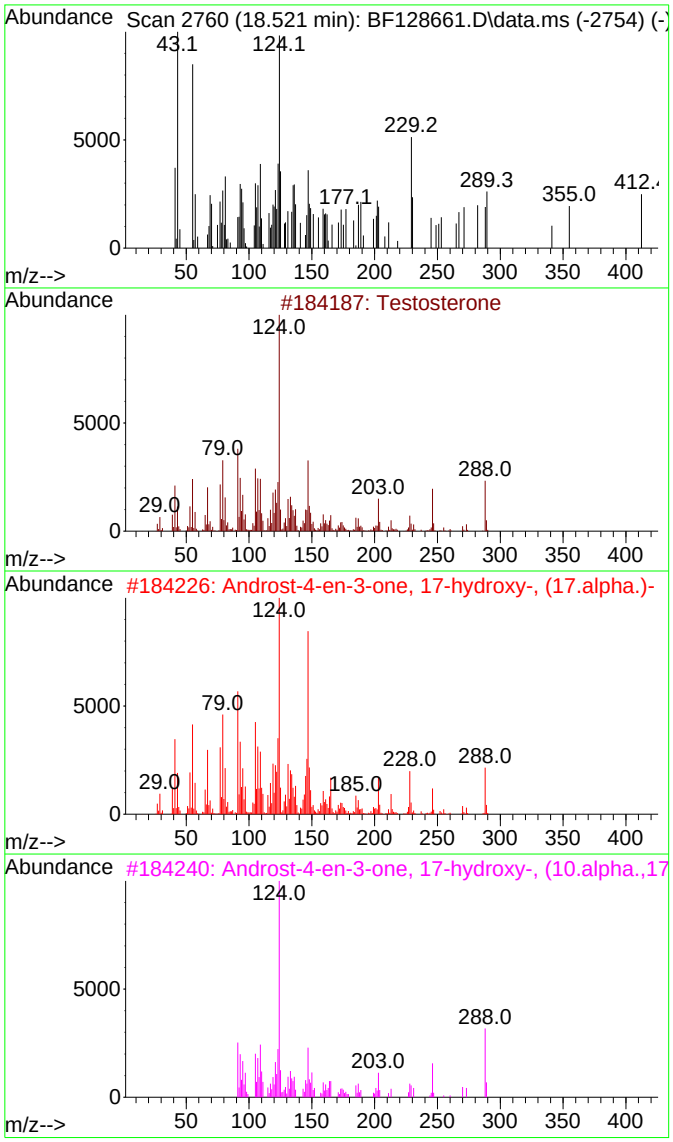
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

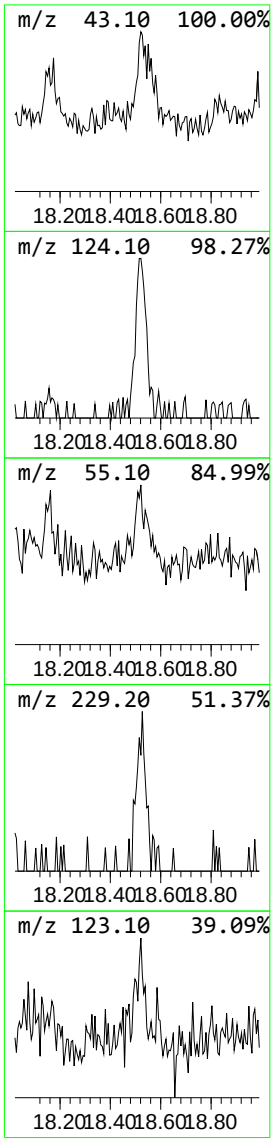
****

Peak Number 10 unknown18.521 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.521	5.96 ng	144106	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Testosterone	288	C19H28O2	000058-22-0	46
2	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	45
3	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	38
4	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	002847-30-5	27
5	Phenol, 4-methoxy-, acetate	166	C9H10O3	001200-06-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060222\
Data File : BF128661.D
Acq On : 03 Jun 2022 02:38
Operator : CG\JU
Sample : N2989-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P015-SS008-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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-...	5.034	3.5	ng	91206	1	6.822	521255	20.0
unknown12.668	12.668	3.0	ng	101865	4	11.351	668680	20.0
Acetic acid n-o...	13.910	4.3	ng	133114	5	13.992	616379	20.0
Triphenylphosph...	14.086	6.4	ng	197335	5	13.992	616379	20.0
1-Propene, 3-(2...	14.127	2.2	ng	67100	5	13.992	616379	20.0
Methadone N-oxide	14.168	3.1	ng	97002	5	13.992	616379	20.0
Eicosane	15.933	2.2	ng	53316	6	15.457	483307	20.0
Hexacosane	17.027	2.6	ng	64145	6	15.457	483307	20.0
2-Isopropenyl-4...	17.262	4.7	ng	113106	6	15.457	483307	20.0
unknown18.521	18.521	6.0	ng	144106	6	15.457	483307	20.0