LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133573.D
Acq On : 05 Jun 2023 19:09
Operator : CG\JU
Sample : 02986-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-15-0A

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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	14	20	32	rVB	46229	70030	2.29%	0.329%
2	5.051	498	504	512	rVB	104708	138628	4.54%	0.651%
3	5.446	566	571	574	rBV	3000662	3030002	99.16%	14.227%
4	6.457	738	743	746	rBV	2851820	3055537	100.00%	14.347%
5	6.834	803	807	810	rBV	1031534	793137	25.96%	3.724%
6	7.398	898	903	906	rBV	2024443	1878369	61.47%	8.820%
7	8.116	1021	1025	1028	rBV	1289425	985692	32.26%	4.628%
8	9.192	1204	1208	1211	rBV	3750185	2994503	98.00%	14.061%
9	9.869	1320	1323	1327	rVB	1177472	929815	30.43%	4.366%
10	10.169	1369	1374	1383	rBV2	16737	48679	1.59%	0.229%
11	10.586	1441	1445	1448	rBV	158051	135052	4.42%	0.634%
12	10.657	1453	1457	1460	rBV	1986454	1719733	56.28%	8.075%
13	11.357	1572	1576	1579	rBV	1093422	871162	28.51%	4.091%
14	11.886	1662	1666	1670	rBV	141980	138336	4.53%	0.650%
15	12.945	1842	1846	1850	rBV	2697271	2566949	84.01%	12.053%
16	13.892	2002	2007	2021	rBV2	70533	236790	7.75%	1.112%
17	13.998	2021	2025	2029	rVB	786656	684755	22.41%	3.215%
18	14.316	2076	2079	2083	rVB	88917	73354	2.40%	0.344%
19	14.474	2104	2106	2110	rVB	63681	57913	1.90%	0.272%
20	14.533	2112	2116	2131	rVV4	116485	253717	8.30%	1.191%
21	14.763	2152	2155	2157	rBV	67384	70549	2.31%	0.331%
22	15.121	2213	2216	2220	rVB2	40084	43501	1.42%	0.204%
23	15.457	2269	2273	2277	rBV	426734	520919	17.05%	2.446%

Sum of corrected areas: 21297122

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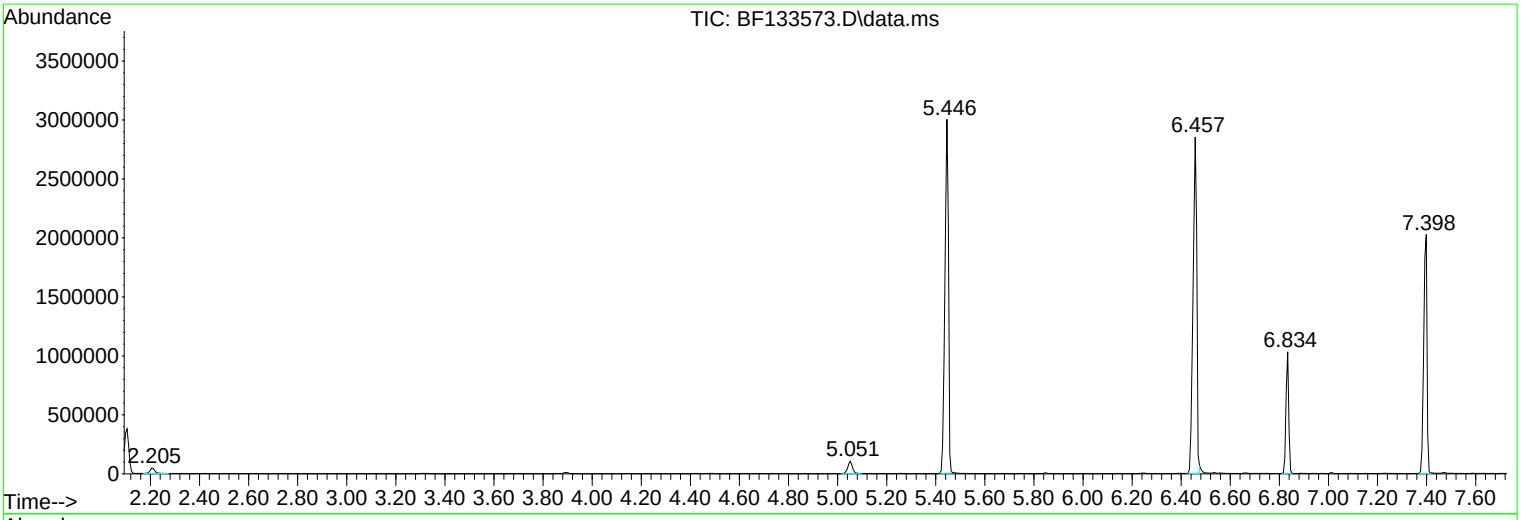
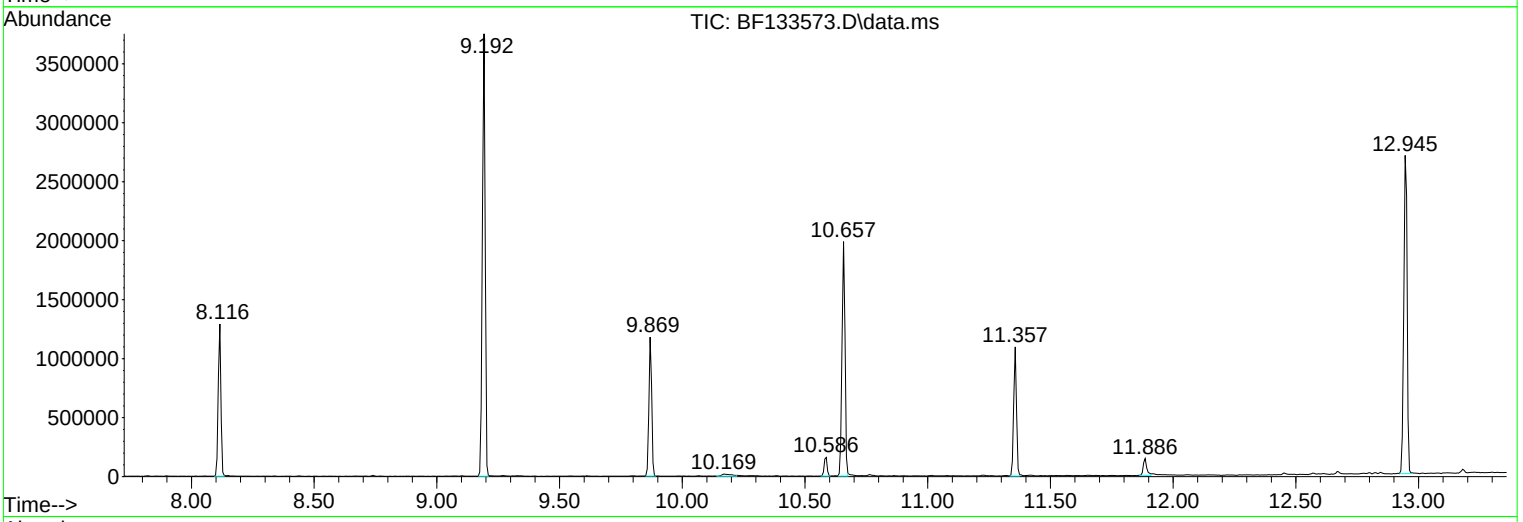
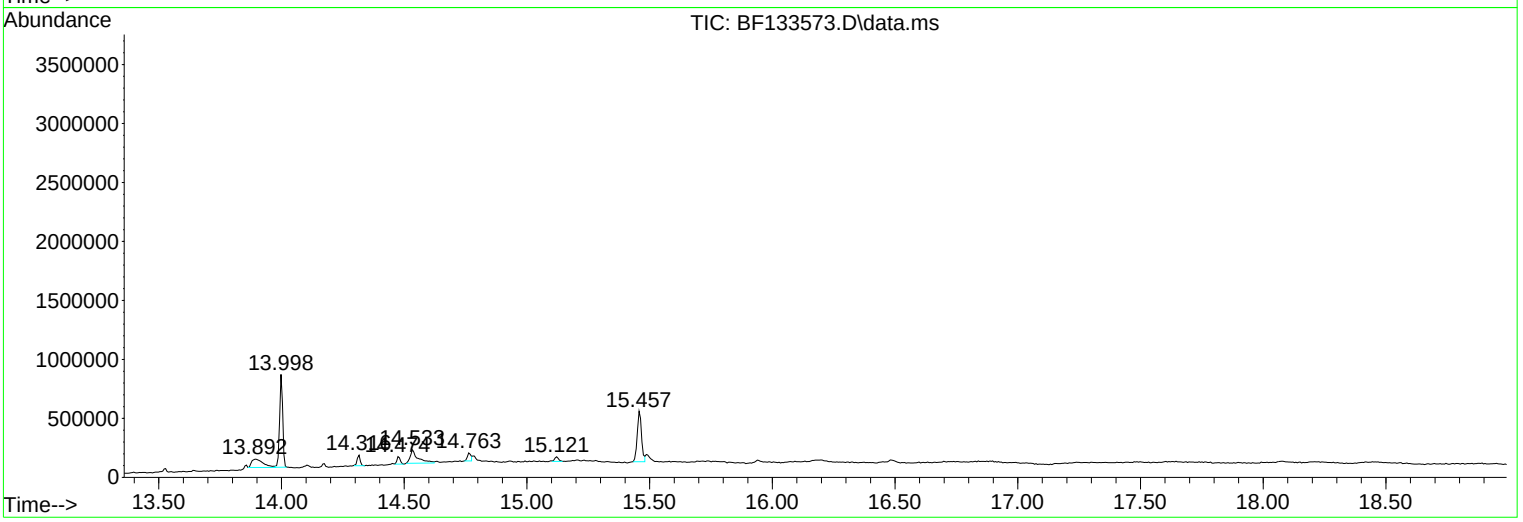
ClientSampleId :
TP-15-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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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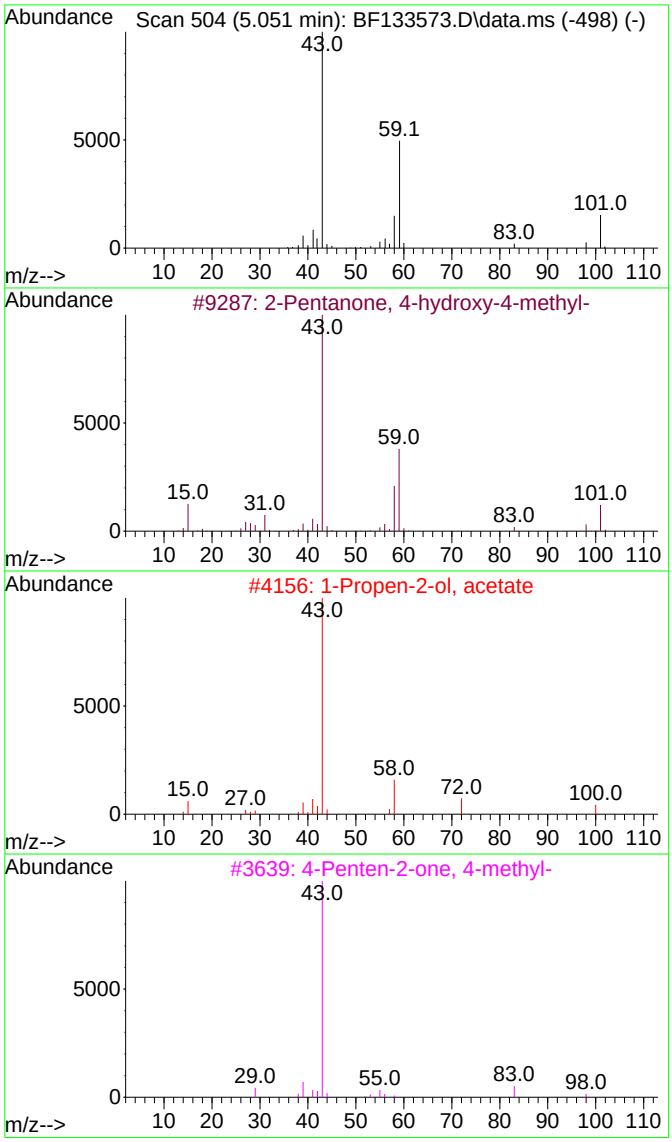
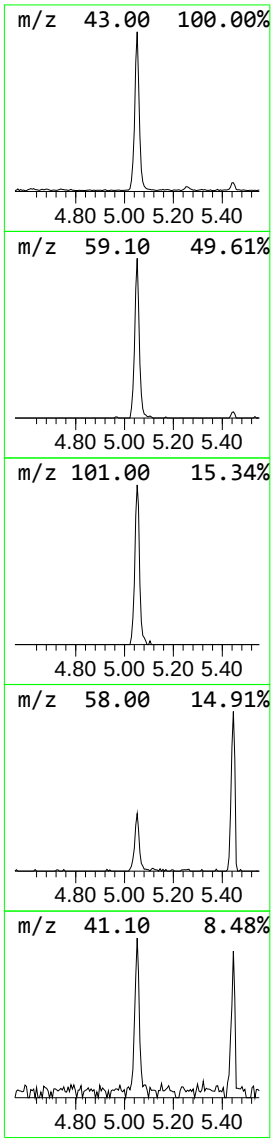
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	3.50 ng	138628	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Data File : BF133573.D
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Sample : 02986-07
Misc :
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Instrument :
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ClientSampleId :
TP-15-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

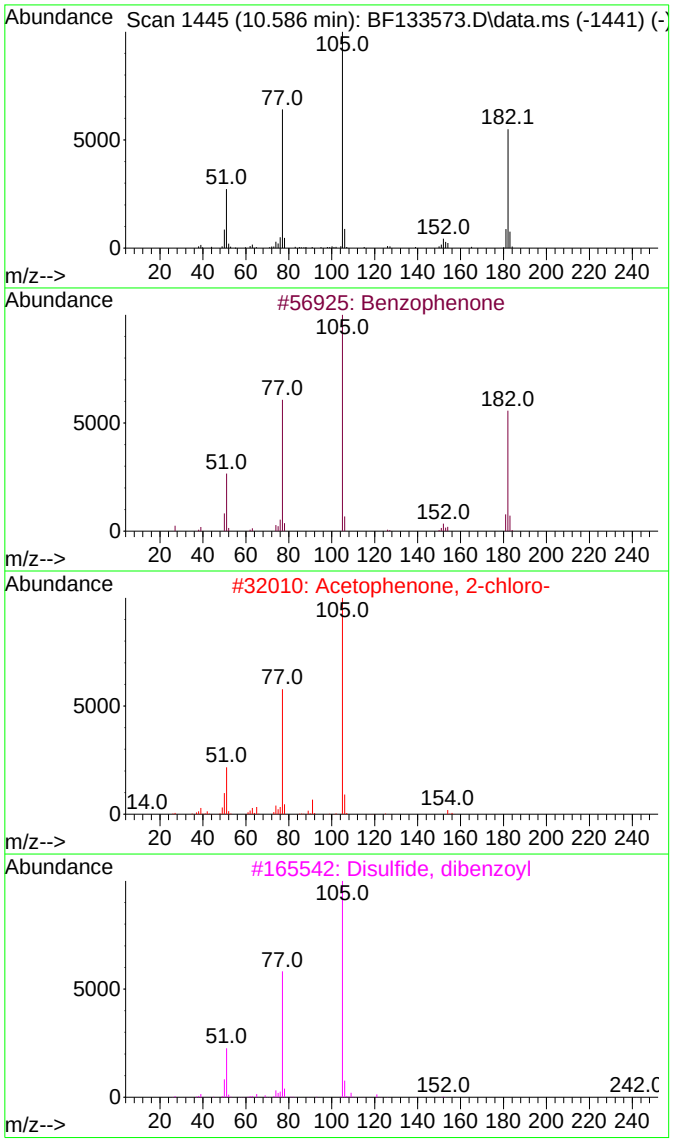
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

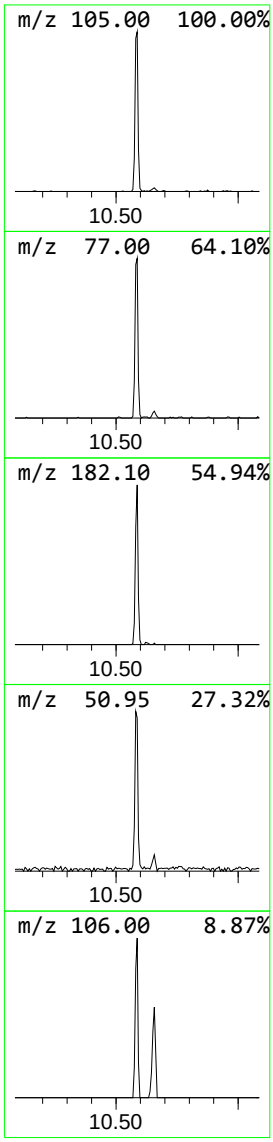
****

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	2.90 ng	135052	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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Acq On : 05 Jun 2023 19:09
Operator : CG\JU
Sample : 02986-07
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-15-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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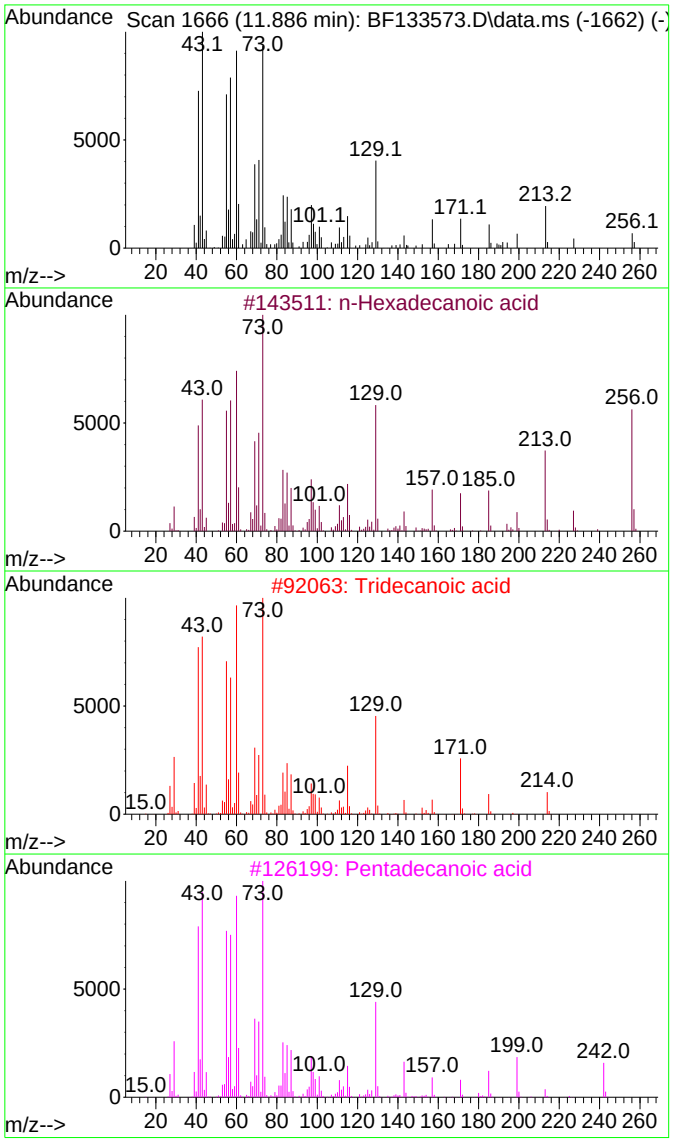
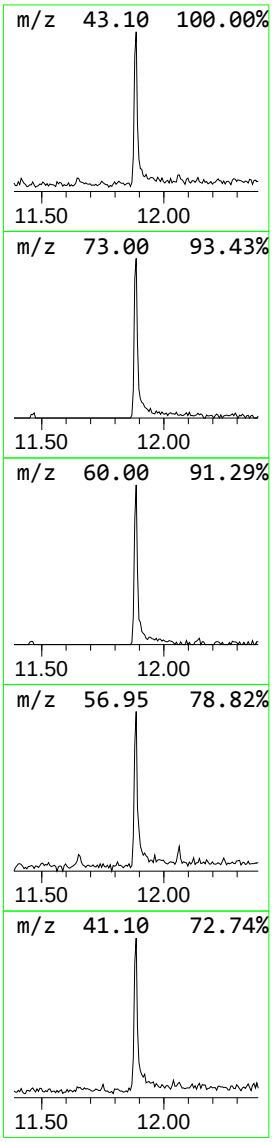
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.18 ng	138336	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Data File : BF133573.D
Acq On : 05 Jun 2023 19:09
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Sample : 02986-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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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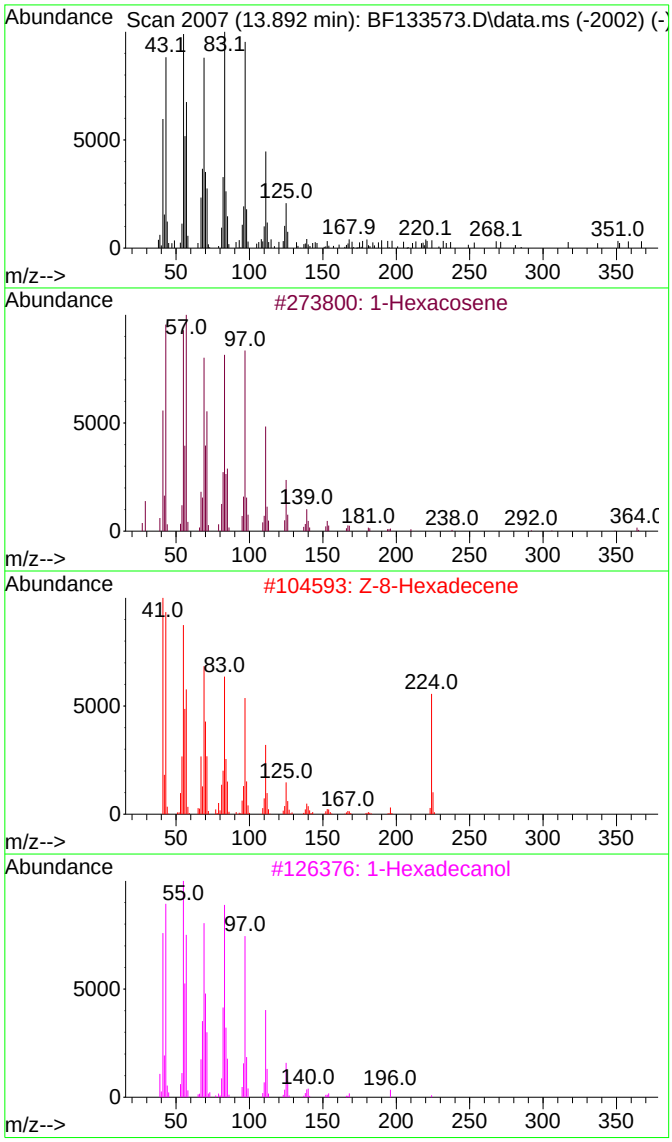
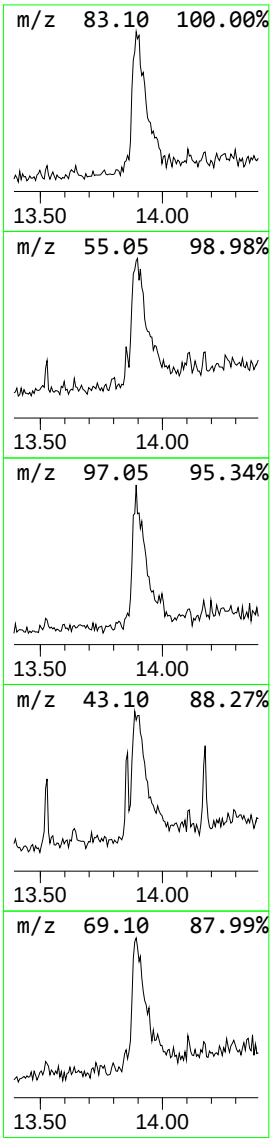
Peak Number 4 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	6.92 ng	236790	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	Z-8-Hexadecene	224	C16H32	1000130-87-5	89
3	1-Hexadecanol	242	C16H34O	036653-82-4	87
4	1-Octadecanol	270	C18H38O	000112-92-5	70
5	1-Nonadecene	266	C19H38	018435-45-5	64





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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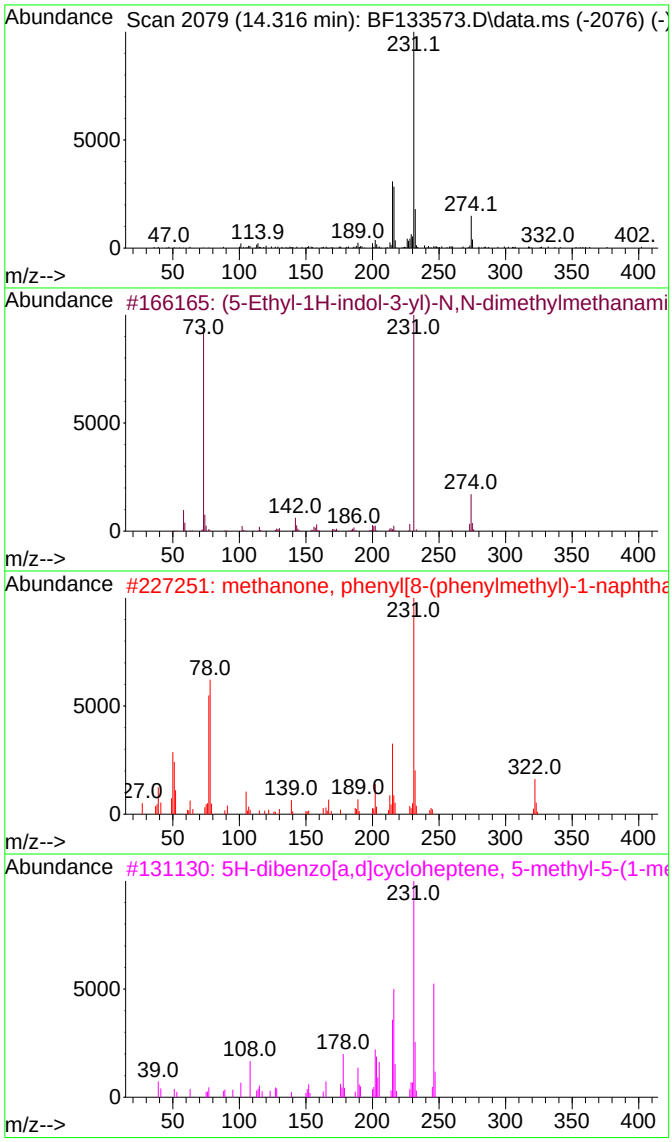
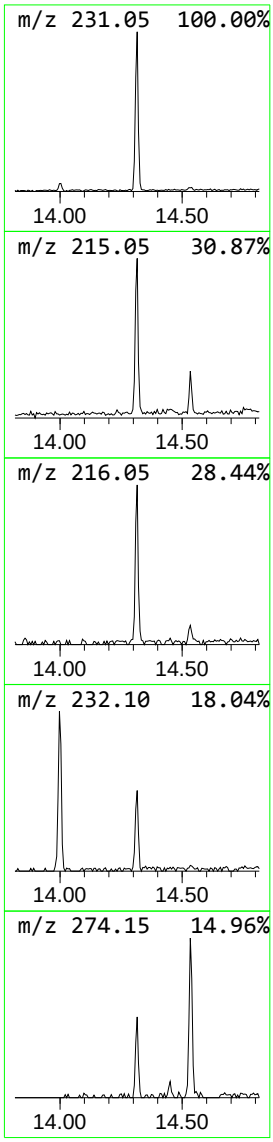
Peak Number 5 unknown14.316 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.316	2.14 ng	73354	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(5-Ethyl-1H-indol-3-yl)-N,N-dime...	274	C16H26N2Si	074367-52-5	47
2	methanone, phenyl[8-(phenylmethy...	322	C24H18O	1000402-34-2	45
3	5H-dibenzo[a,d]cycloheptene, 5-m...	246	C19H18	1000396-58-1	42
4	naphtho[1,2-d]thiazole, 4,5-dihy...	231	C13H13NOS	1000401-02-8	40
5	3-(2-Bromo-4,5-dimethoxyphenyl)-...	310	C12H11BrN2O3	1000459-09-2	39





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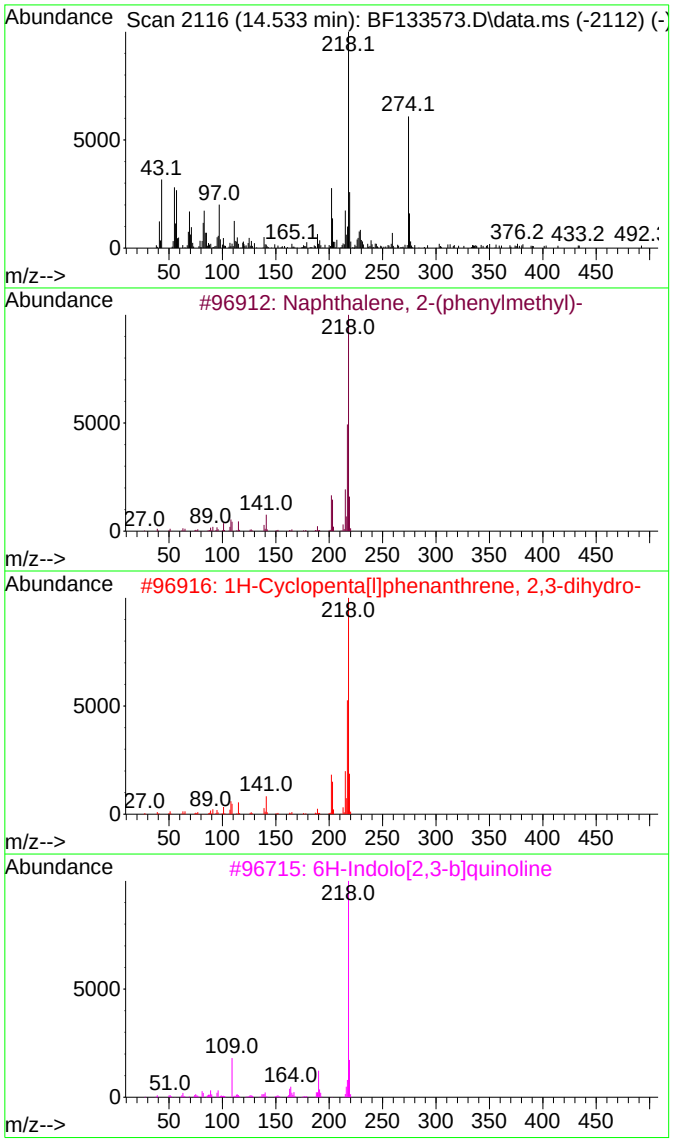
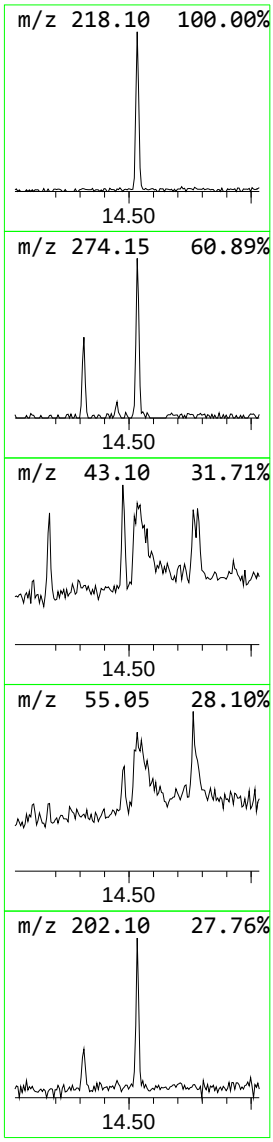
Peak Number 6 unknown14.533 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	7.41 ng	253717	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-(phenylmethyl)-	218	C17H14	000613-59-2	43
2	1H-Cyclopenta[l]phenanthrene, 2,...	218	C17H14	000723-98-8	43
3	6H-Indolo[2,3-b]quinoline	218	C15H10N2	000243-38-9	38
4	l-Valine, n-pentafluoropropionyl...	403	C18H30F5NO3	1000320-88-5	38
5	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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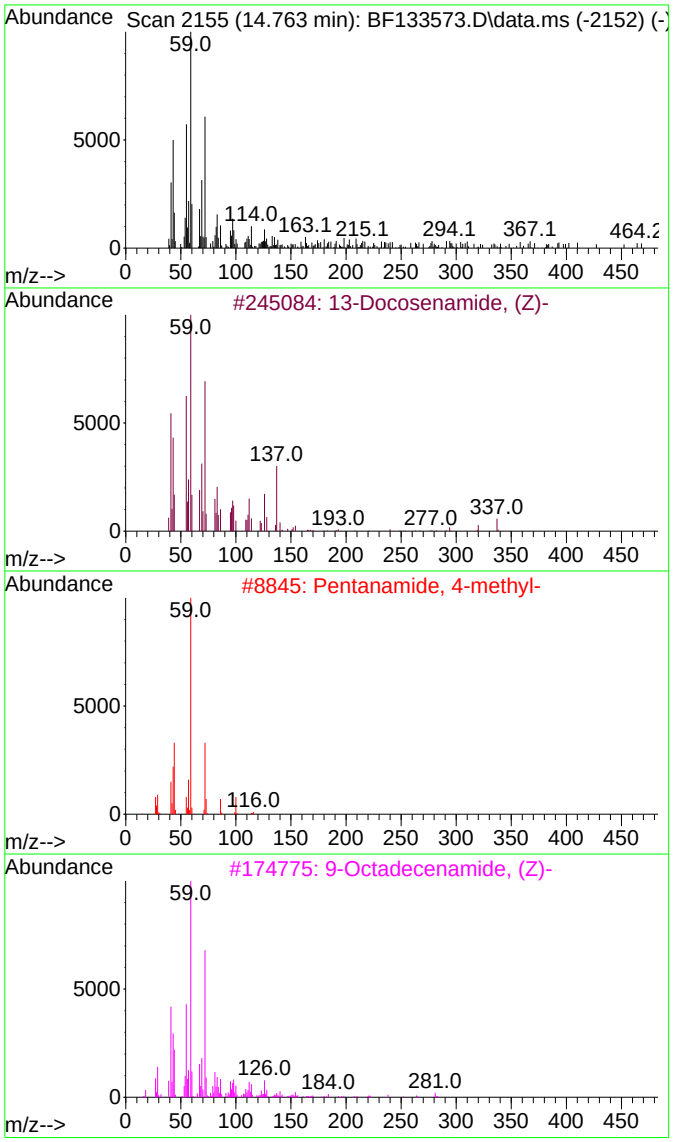
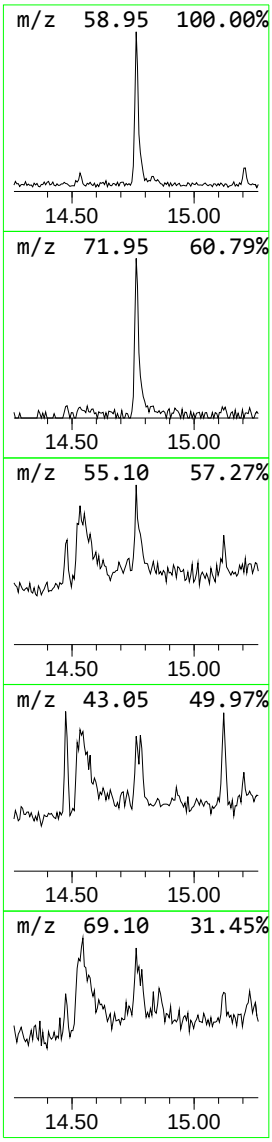
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	2.71 ng	70549	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
2	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38
4	2,4,6,8,9,10-Hexathiatricyclo[3....	358	C10H14O2S6	057274-38-1	38
5	2-Butene, 1-propoxy-, (E)-	114	C7H14O	056052-71-2	14





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	3.5	ng	138628	1	6.834	793137	20.0
Benzophenone	10.586	2.9	ng	135052	3	9.869	929815	20.0
n-Hexadecanoic ...	11.886	3.2	ng	138336	4	11.357	871162	20.0
1-Hexacosene	13.892	6.9	ng	236790	5	13.998	684755	20.0
unknown14.316	14.316	2.1	ng	73354	5	13.998	684755	20.0
unknown14.533	14.533	7.4	ng	253717	5	13.998	684755	20.0
13-Docosenamide...	14.763	2.7	ng	70549	6	15.457	520919	20.0