LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060923\
Data File : BF133683.D
Acq On : 09 Jun 2023 19:01
Operator : CG\JU
Sample : 03039-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB31A

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	499	503	511	rVB	80330	101966	5.34%	0.809%
2	5.451	567	572	575	rBV	1663615	1494269	78.32%	11.856%
3	6.463	739	744	747	rBV	1615332	1571426	82.37%	12.468%
4	6.840	804	808	811	rBV	652594	574676	30.12%	4.560%
5	7.398	899	903	906	rBV	1171500	990398	51.91%	7.858%
6	8.122	1022	1026	1029	rBV	905127	709427	37.19%	5.629%
7	9.198	1205	1209	1212	rBV	2343742	1907820	100.00%	15.137%
8	9.875	1321	1324	1328	rBV	897485	753895	39.52%	5.982%
9	10.592	1442	1446	1449	rBV	348458	285805	14.98%	2.268%
10	10.669	1455	1459	1462	rBV	1059098	994880	52.15%	7.894%
11	10.898	1495	1498	1503	rVB	29699	23598	1.24%	0.187%
12	11.369	1574	1578	1581	rBV	782996	693901	36.37%	5.506%
13	11.892	1664	1667	1670	rBV2	73838	69455	3.64%	0.551%
14	12.580	1780	1784	1790	rBV	32818	31681	1.66%	0.251%
15	12.957	1844	1848	1851	rBV	1678336	1442528	75.61%	11.445%
16	13.886	2002	2006	2009	rVB5	23081	33343	1.75%	0.265%
17	14.010	2023	2027	2030	rBV	490722	426677	22.36%	3.385%
18	14.792	2158	2160	2163	rVB2	38776	39235	2.06%	0.311%
19	14.933	2182	2184	2187	rVB	56269	44366	2.33%	0.352%
20	15.127	2215	2217	2220	rVB	40111	34229	1.79%	0.272%
21	15.480	2273	2277	2281	rBV	303133	328055	17.20%	2.603%
22	15.945	2354	2356	2362	rVB2	40318	52119	2.73%	0.414%

Sum of corrected areas: 12603749

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060923\
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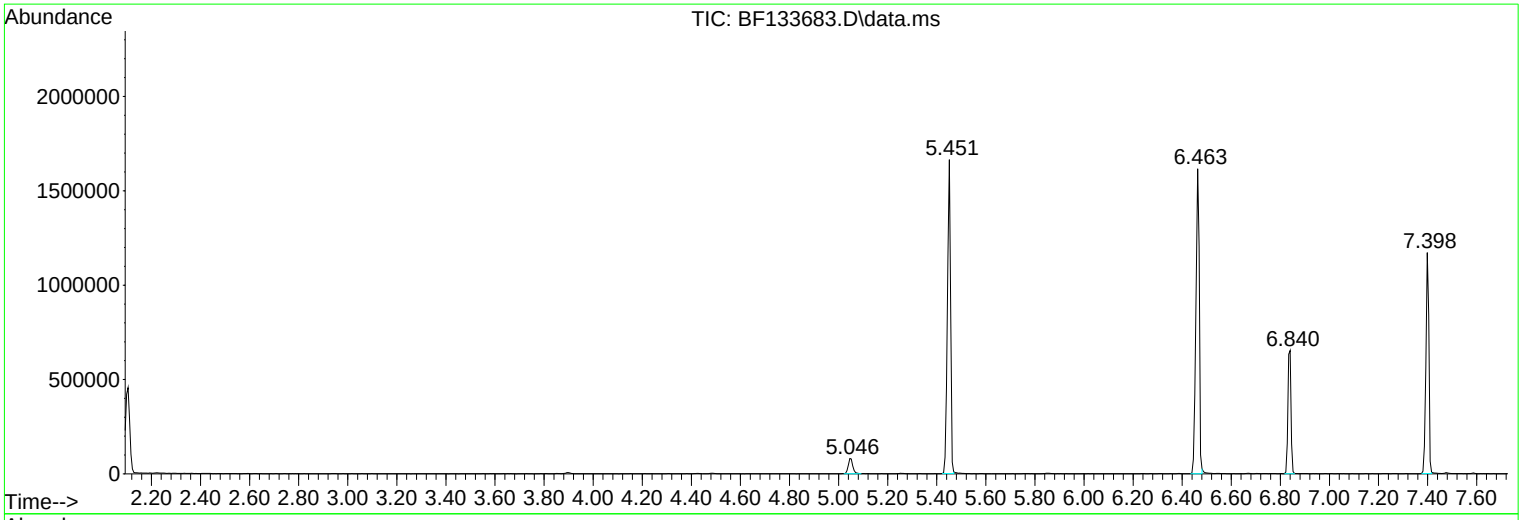
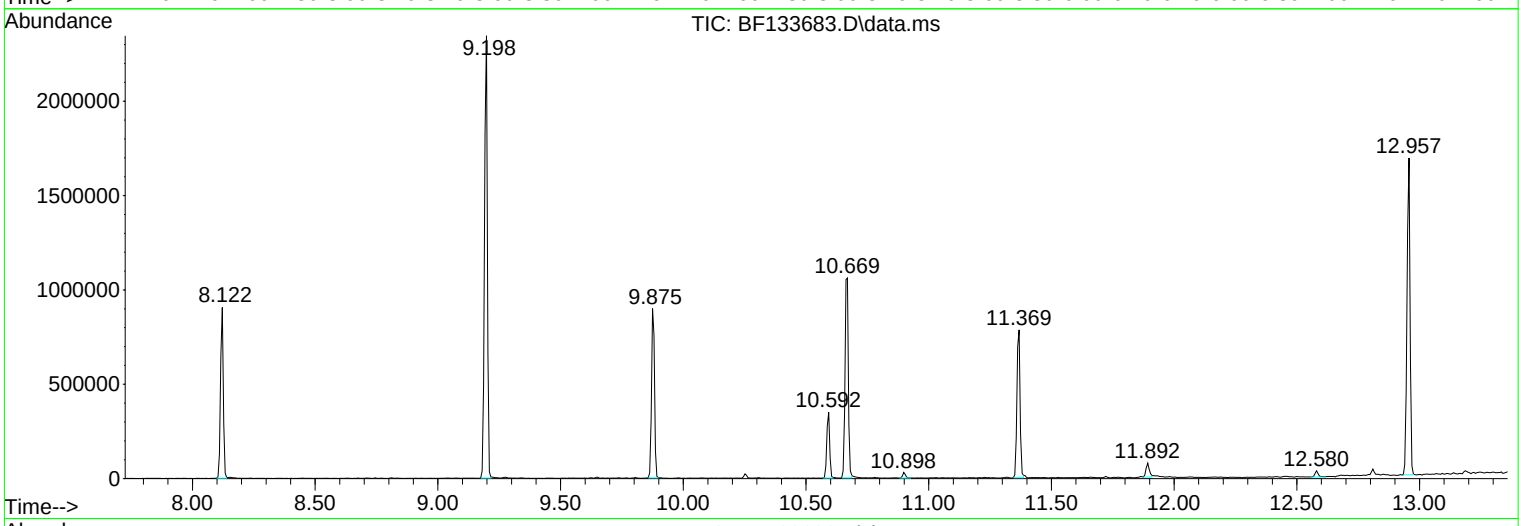
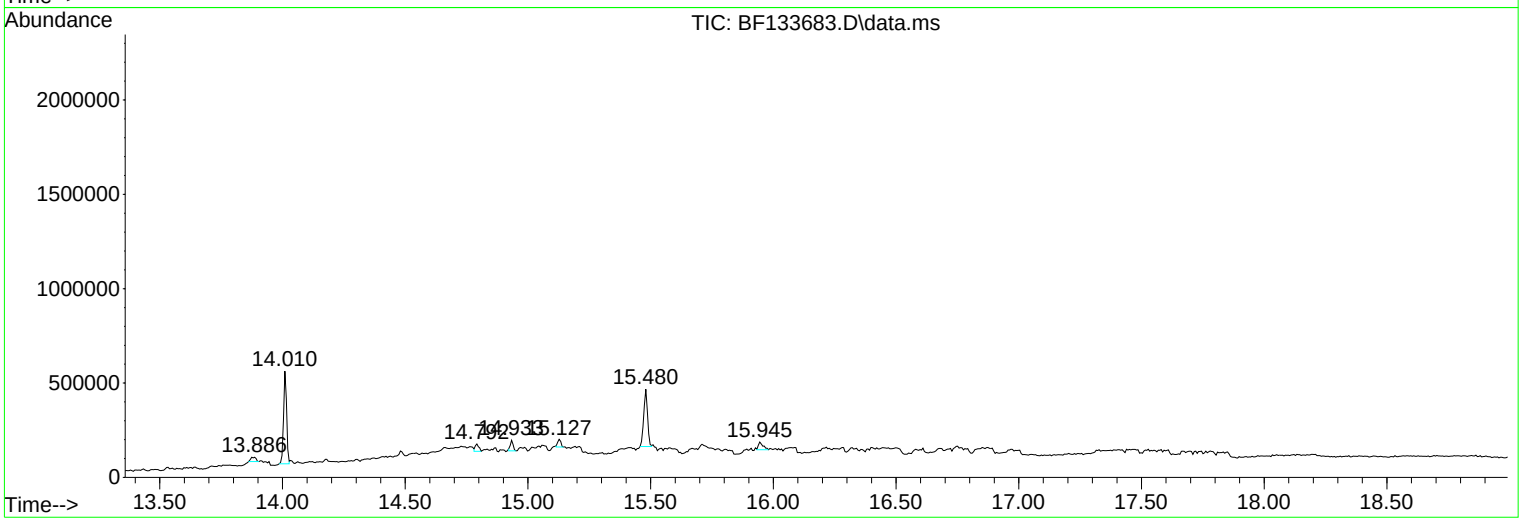
Instrument :
BNA_F
ClientSampleId :
SB31A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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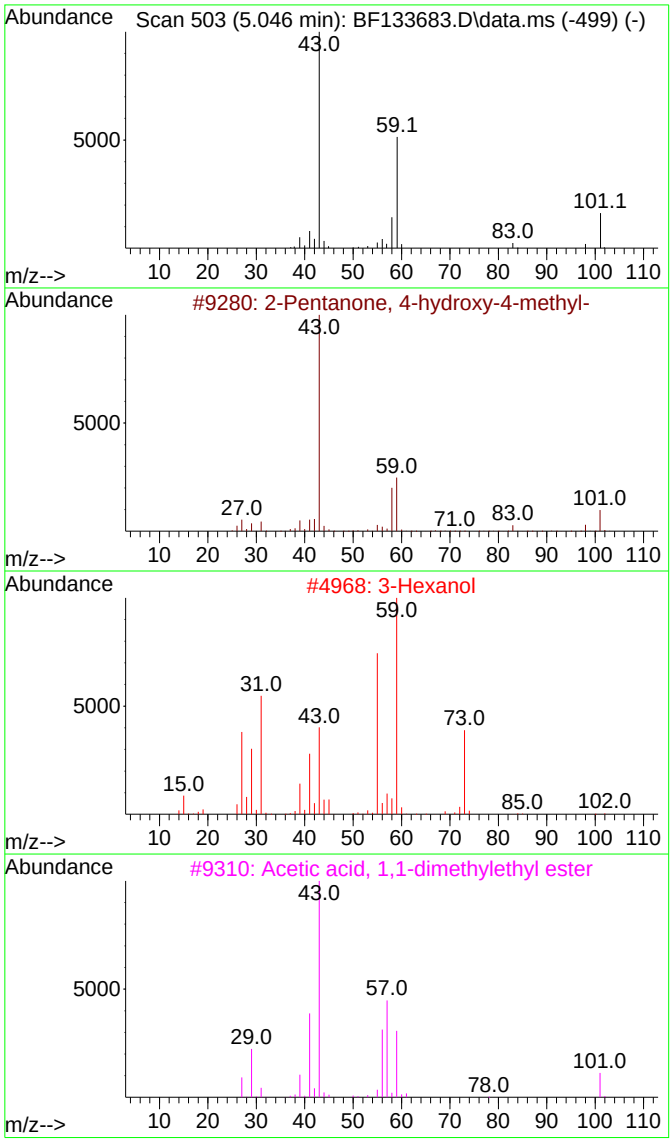
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

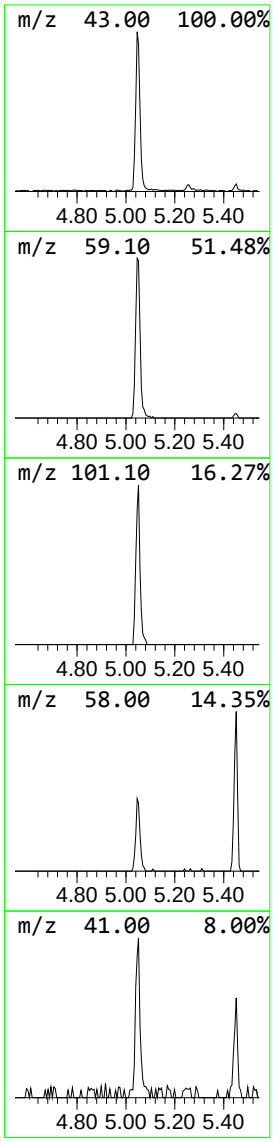
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	3.55 ng	101966	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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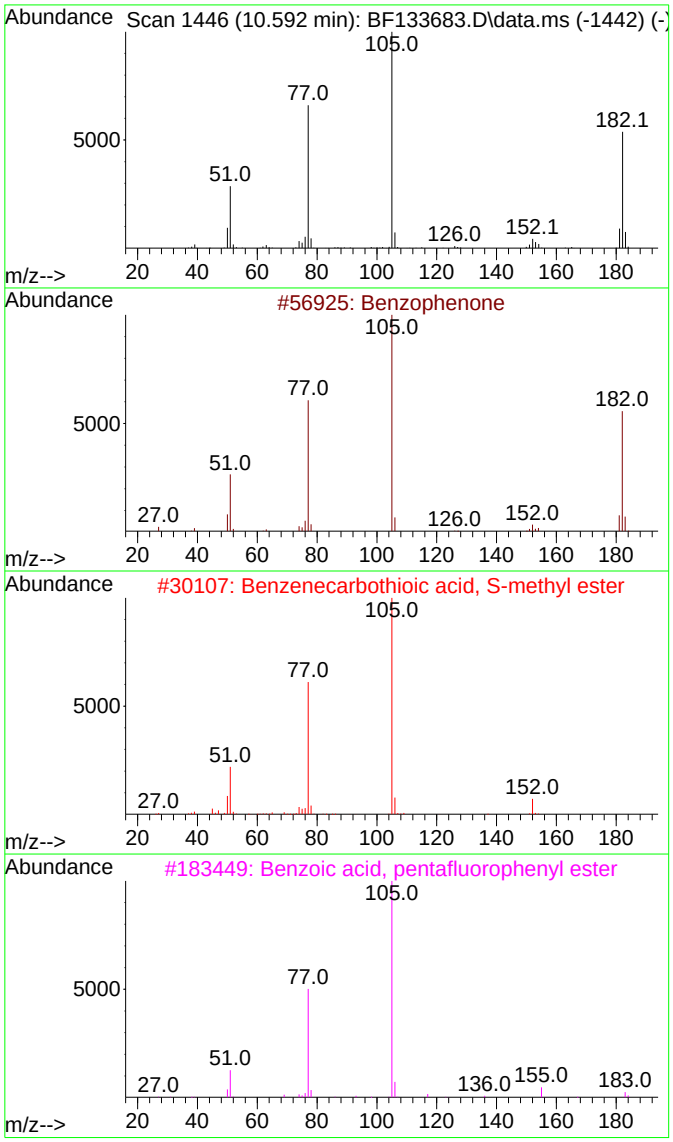
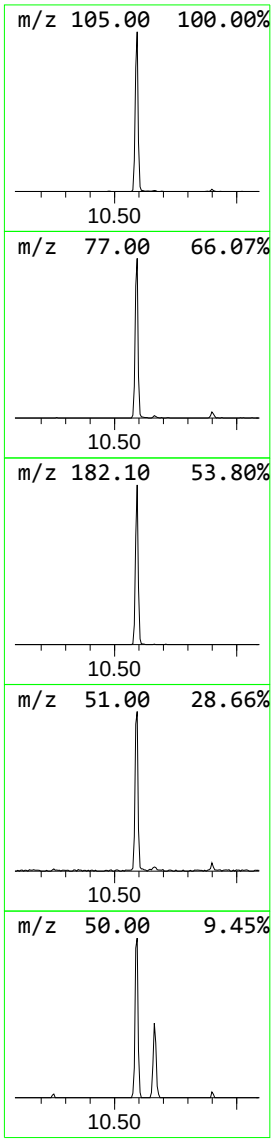
Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.592	7.58 ng	285805	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
4	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
5	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47





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Sample : 03039-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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TIC Library : C:\Database\NIST20.L
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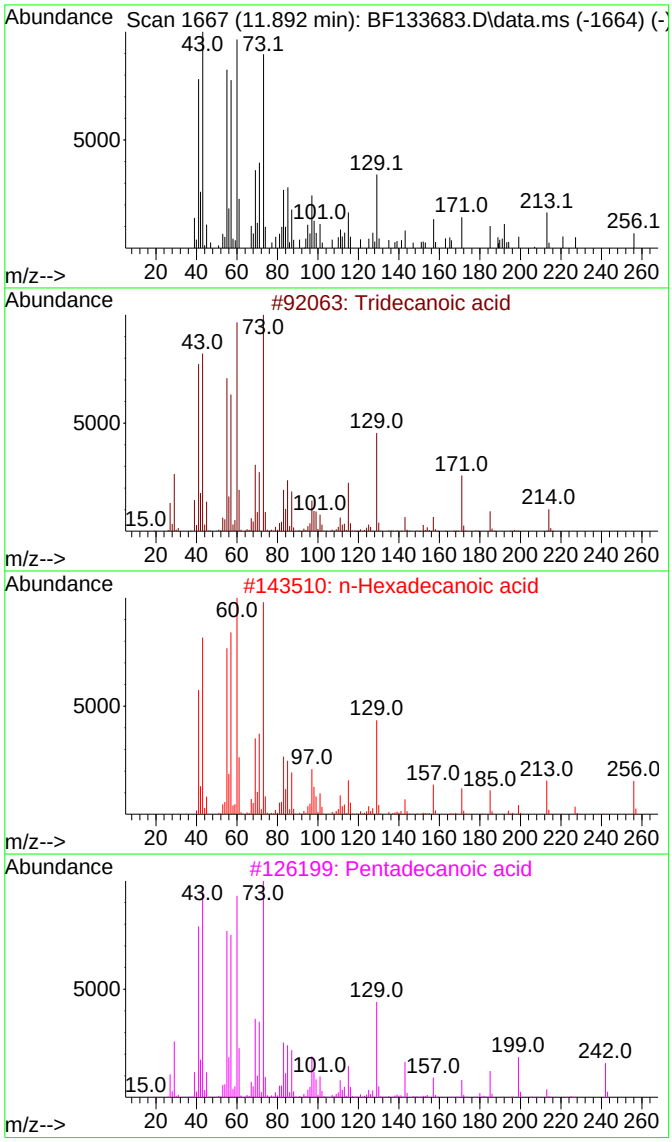
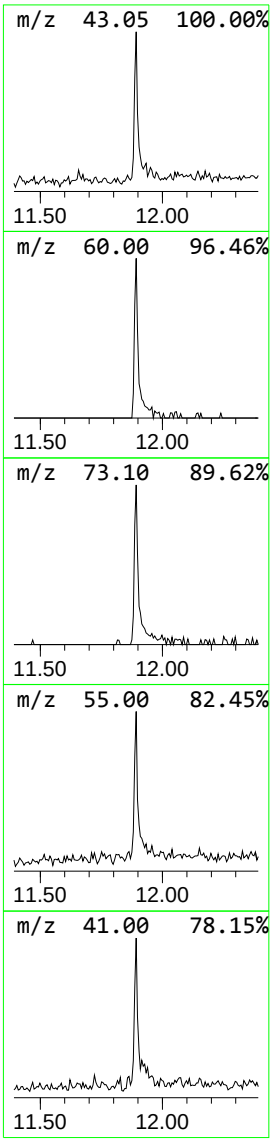
Peak Number 3 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.00 ng	69455	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	92
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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TIC Library : C:\Database\NIST20.L
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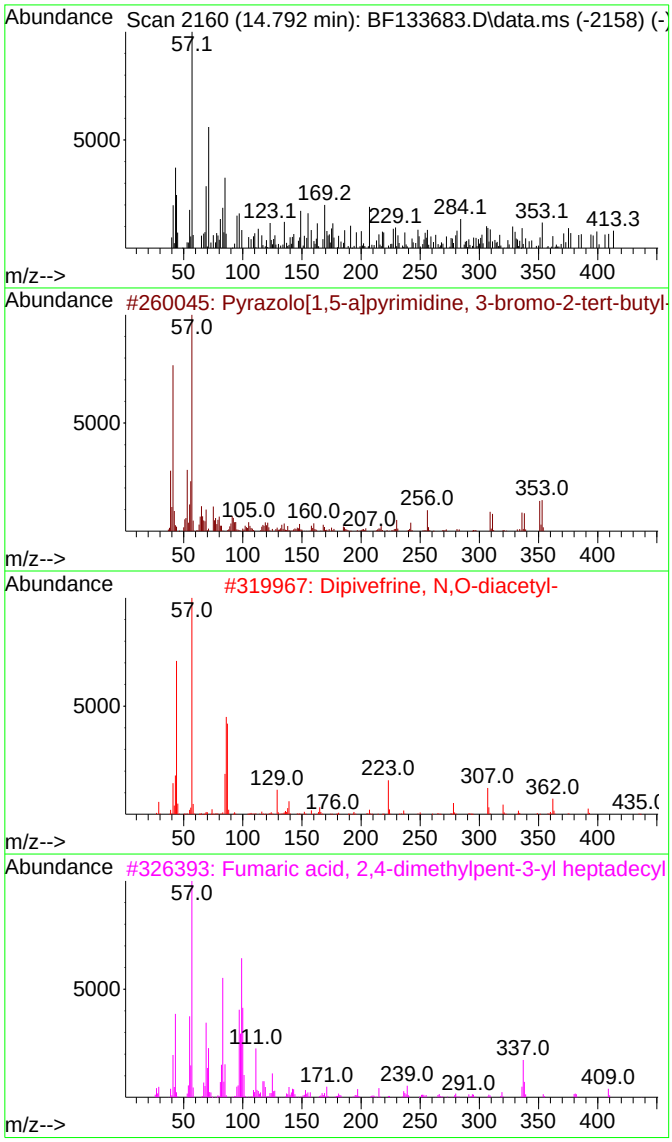
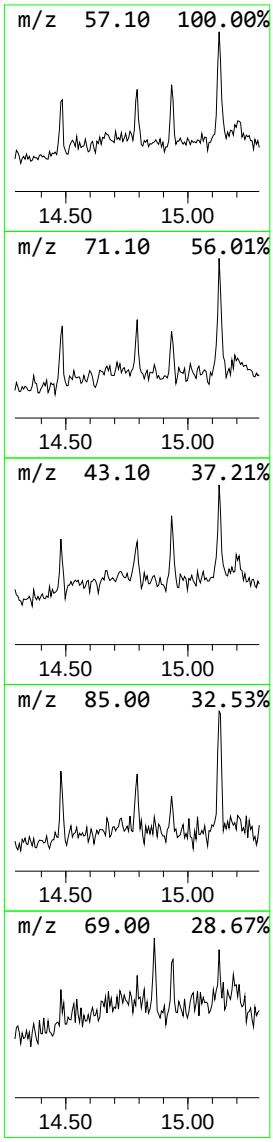
Peak Number 4 unknown14.792 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	2.39 ng	39235	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo[1,5-a]pyrimidine, 3-bro...	351	C12H13BrF3N3O	1000265-06-8	7
2	Dipivefrine, N,O-diacetyl-	435	C23H33NO7	1010417-50-4	4
3	Fumaric acid, 2,4-dimethylpent-3...	452	C28H52O4	1000348-55-8	2
4	Hexanoic acid, 2-(4-iodo-1-methy...	434	C14H19IN4O4	1000276-82-0	2
5	2-(2-Benzothiazolyl)-4-(3-nitrob...	375	C20H13N3O3S	1000224-40-9	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060923\
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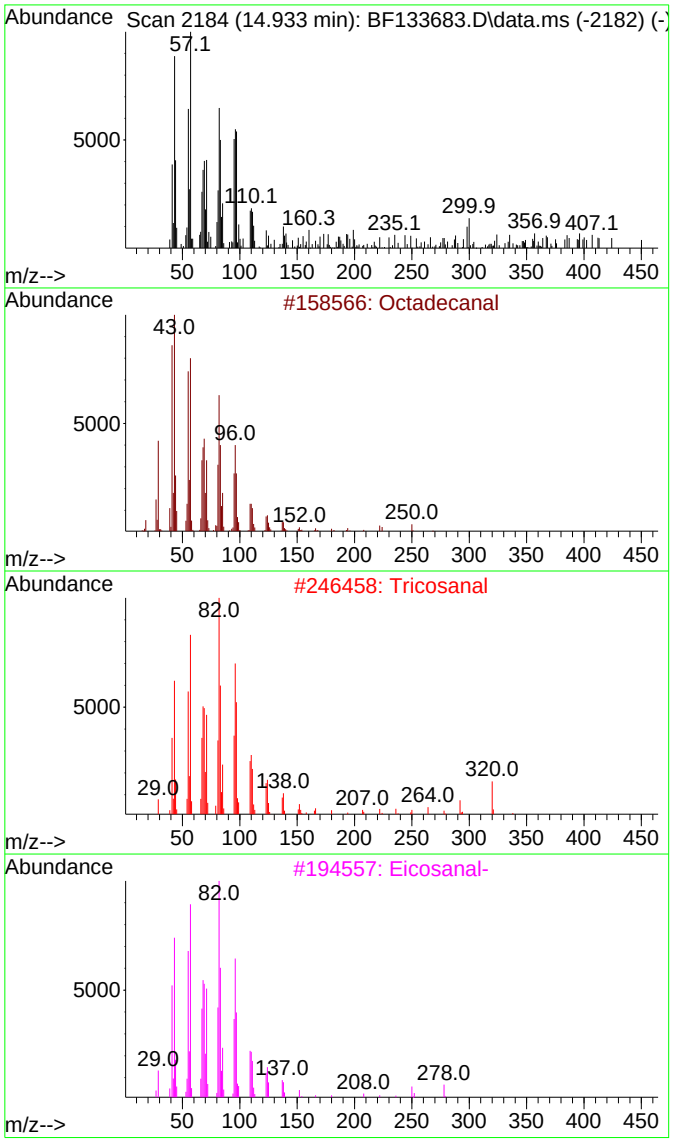
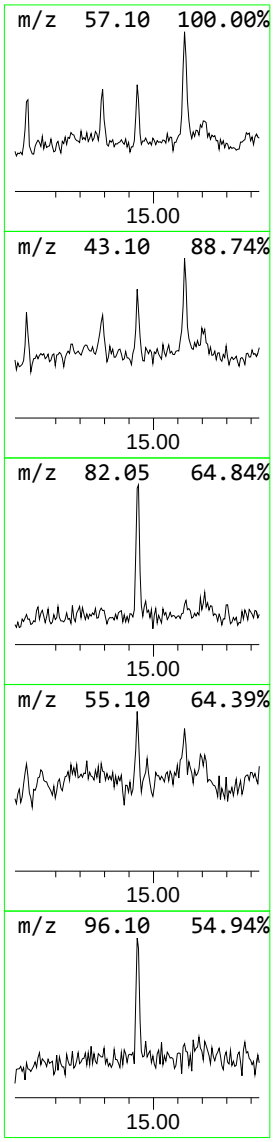
Peak Number 5 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	2.70 ng	44366	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	89
2	Tricosanal	338	C23H46O	072934-02-2	89
3	Eicosanal-	296	C20H40O	002400-66-0	50
4	Hexacosanal	380	C26H52O	026627-85-0	50
5	1,19-Eicosadiene	278	C20H38	014811-95-1	50





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TIC Library : C:\Database\NIST20.L
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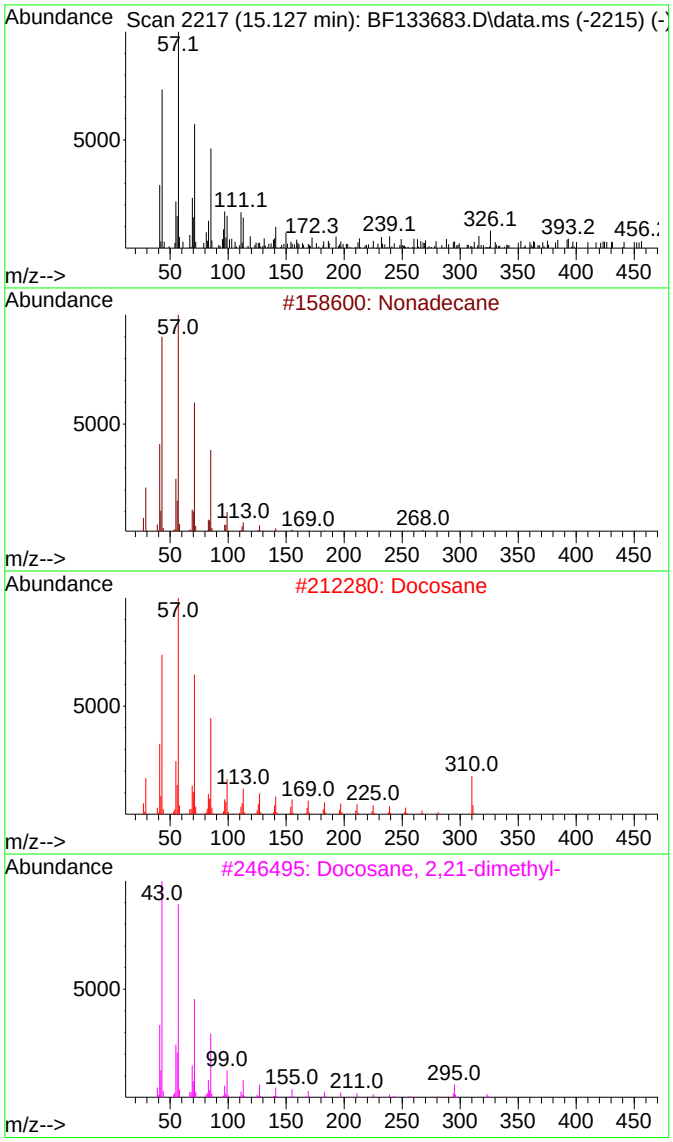
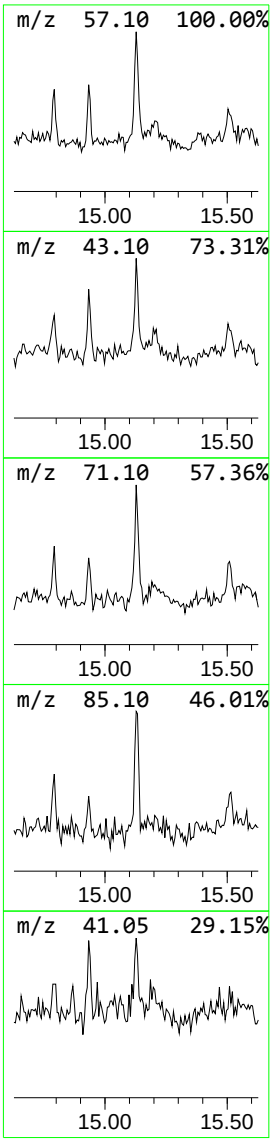
Peak Number 6 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.09 ng	34229	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	89
2	Docosane	310	C22H46	000629-97-0	76
3	Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	76
4	Pentadecane	212	C15H32	000629-62-9	76
5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	76





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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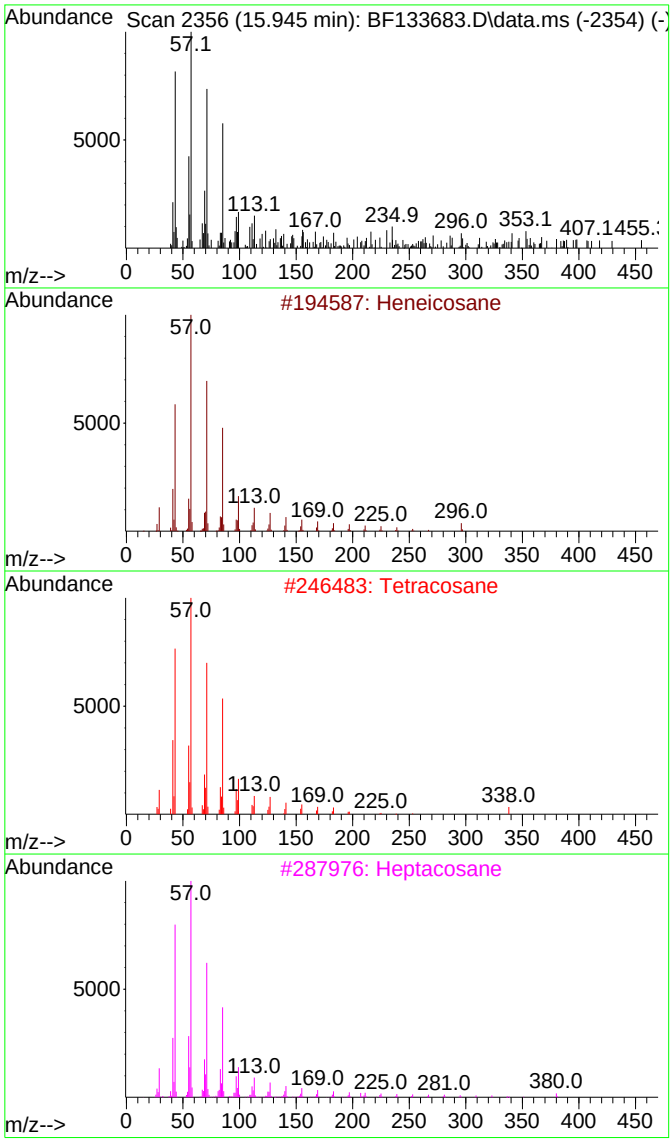
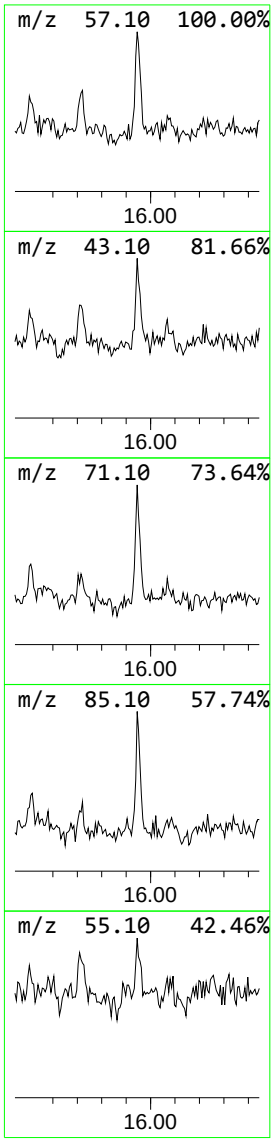
Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	3.18 ng	52119	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Tetracosane	338	C24H50	000646-31-1	93
3	Heptacosane	380	C27H56	000593-49-7	89
4	Hexacosane	366	C26H54	000630-01-3	86
5	Pentadecane	212	C15H32	000629-62-9	83





Tentatively Identified Compound (LSC) summary

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Data File : BF133683.D
Acq On : 09 Jun 2023 19:01
Operator : CG\JU
Sample : 03039-04
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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-...	5.046	3.5	ng	101966	1	6.840	574676	20.0
Benzophenone	10.592	7.6	ng	285805	3	9.875	753895	20.0
Tridecanoic acid	11.892	2.0	ng	69455	4	11.369	693901	20.0
unknown14.792	14.792	2.4	ng	39235	6	15.480	328055	20.0
Octadecanal	14.933	2.7	ng	44366	6	15.480	328055	20.0
Nonadecane	15.127	2.1	ng	34229	6	15.480	328055	20.0
Heneicosane	15.945	3.2	ng	52119	6	15.480	328055	20.0