LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140830.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	24	rVB	1415806	2335859	100.00%	12.922%
2	5.504	574	580	615	rBV	1210630	1730154	74.07%	9.572%
3	6.510	746	751	778	rBV	1346385	1891730	80.99%	10.465%
4	6.857	805	810	818	rBV	394615	490408	20.99%	2.713%
5	7.428	901	907	918	rBV	888820	1220941	52.27%	6.755%
6	7.681	945	950	963	rBV	29697	55107	2.36%	0.305%
7	8.139	1023	1028	1048	rBV	433938	563429	24.12%	3.117%
8	9.216	1205	1211	1221	rBV	1783412	2301502	98.53%	12.732%
9	9.898	1322	1327	1341	rBV	600676	774474	33.16%	4.285%
10	10.610	1443	1448	1457	rBV	123695	163065	6.98%	0.902%
11	10.692	1457	1462	1476	rBV	1036260	1388688	59.45%	7.683%
12	11.392	1575	1581	1588	rBV	586906	796536	34.10%	4.407%
13	11.457	1588	1592	1595	rBV	30788	43351	1.86%	0.240%
14	11.604	1610	1617	1630	rVB7	21532	73285	3.14%	0.405%
15	11.910	1664	1669	1682	rBV	298875	488196	20.90%	2.701%
16	12.621	1783	1790	1798	rBV8	16271	50102	2.14%	0.277%
17	12.698	1798	1803	1815	rVB2	58326	112935	4.83%	0.625%
18	12.974	1844	1850	1855	rBV	1694987	2151762	92.12%	11.904%
19	13.451	1926	1931	1940	rVB	159974	227462	9.74%	1.258%
20	13.863	1996	2001	2009	rBV	111379	167837	7.19%	0.929%
21	14.045	2027	2032	2040	rBV	336228	464637	19.89%	2.570%
22	14.221	2053	2062	2073	rVB6	34124	108033	4.62%	0.598%
23	15.545	2281	2287	2297	rBV	262264	476430	20.40%	2.636%

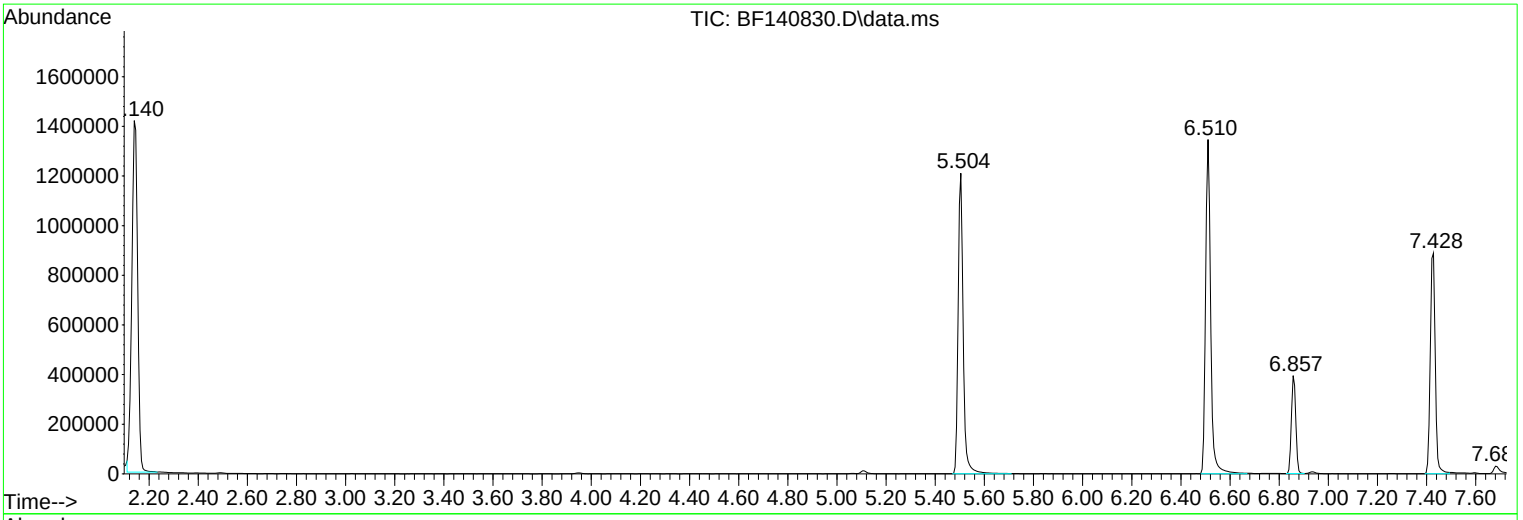
Sum of corrected areas: 18075923

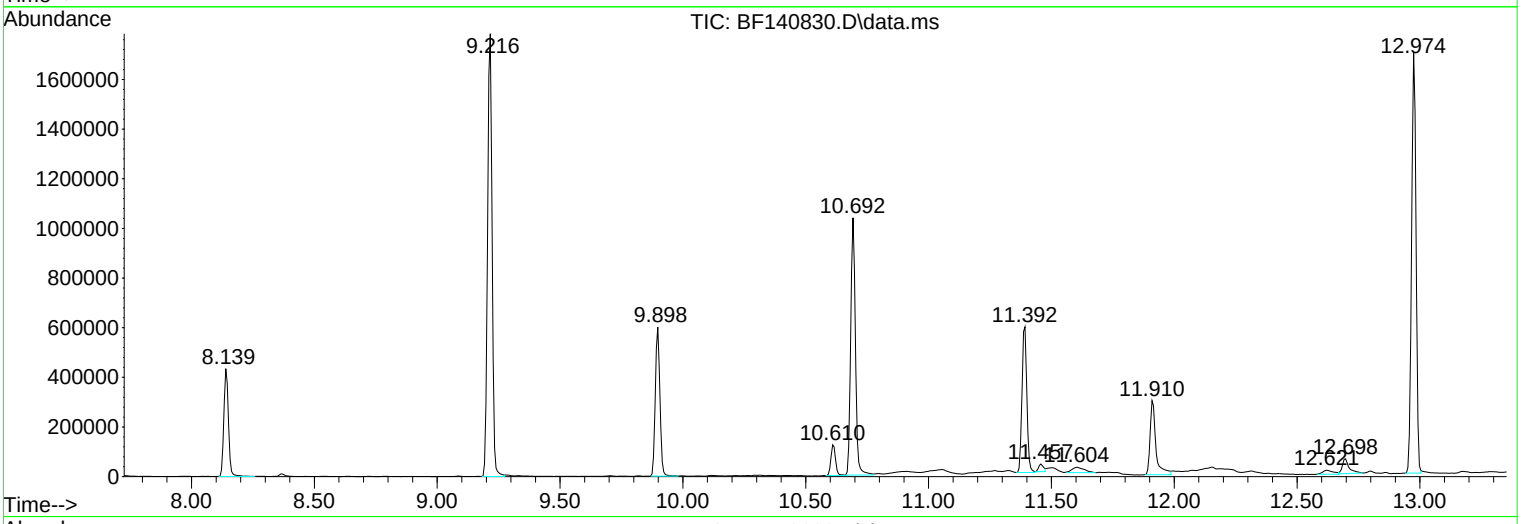
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

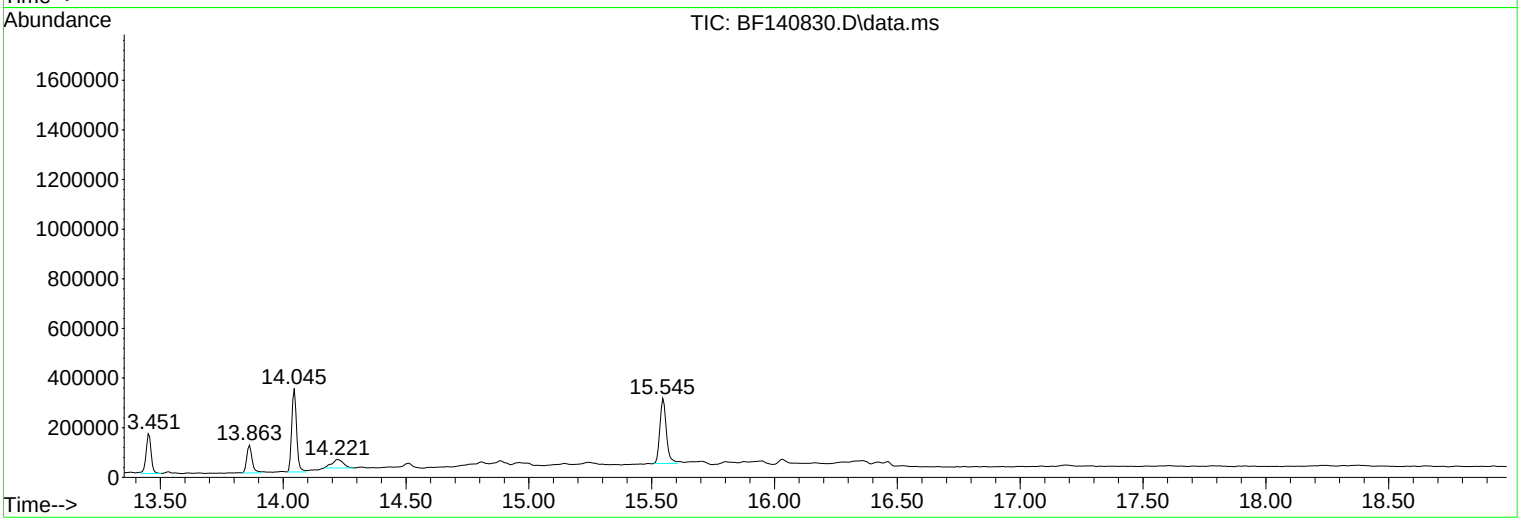
Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

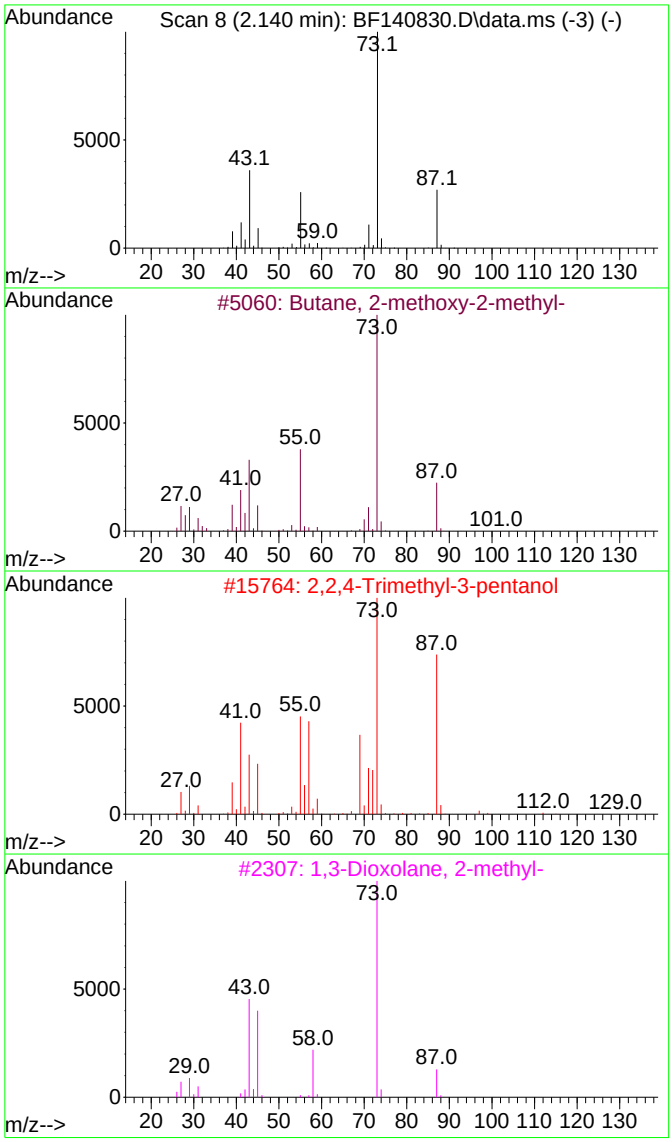
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

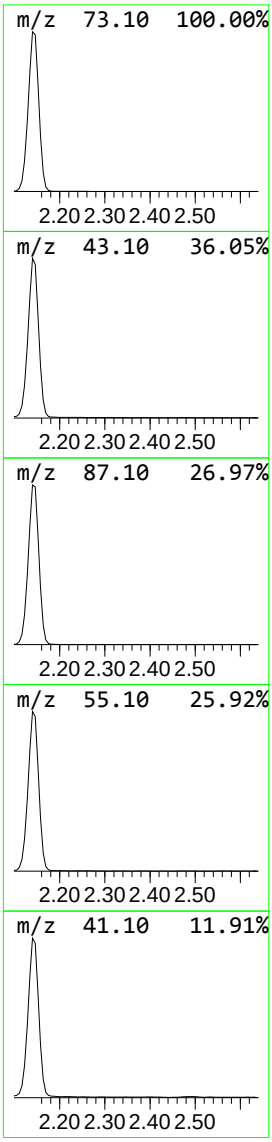
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	95.26 ng	2335860	1,4-Dichlorobenzene-d4	6.857

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

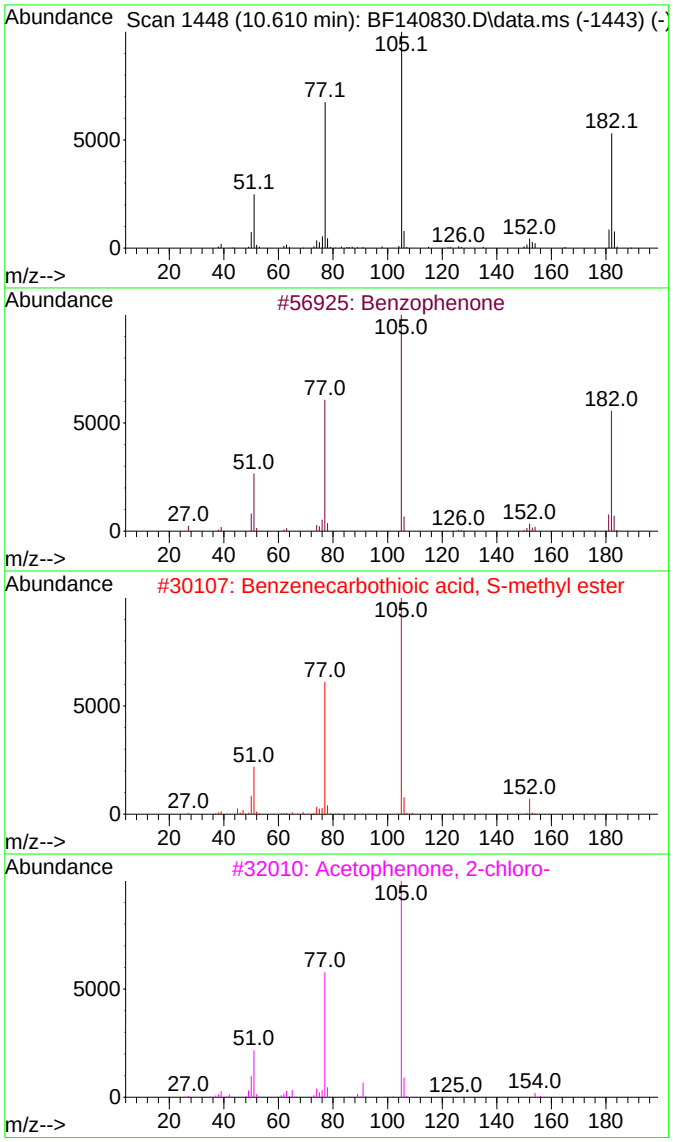
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

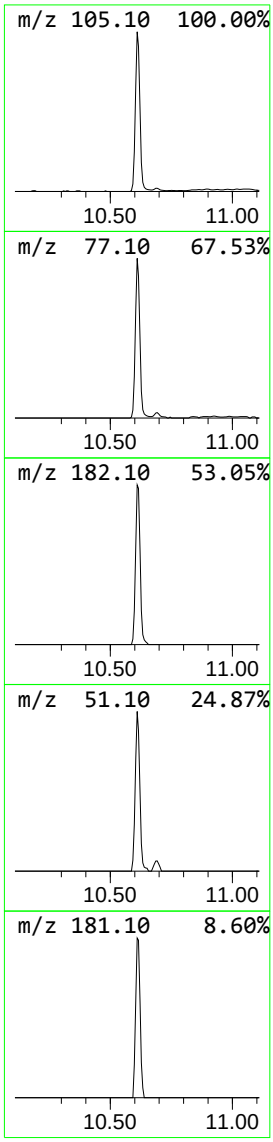
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	4.21 ng	163065	Acenaphthene-d10	9.898

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	49
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5	Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

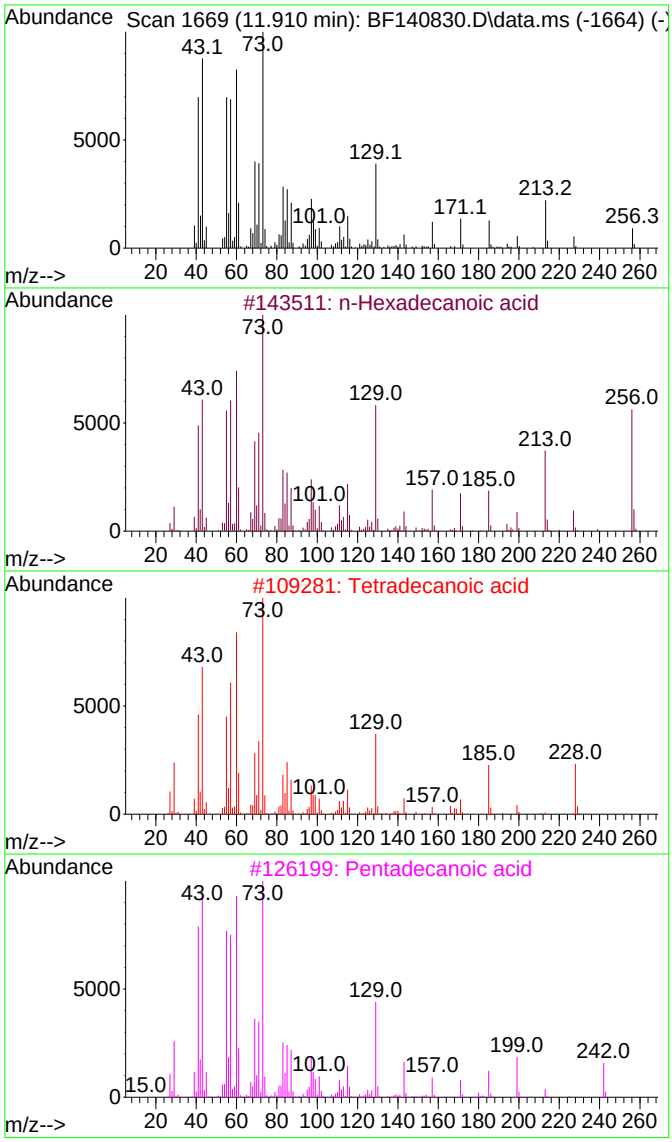
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

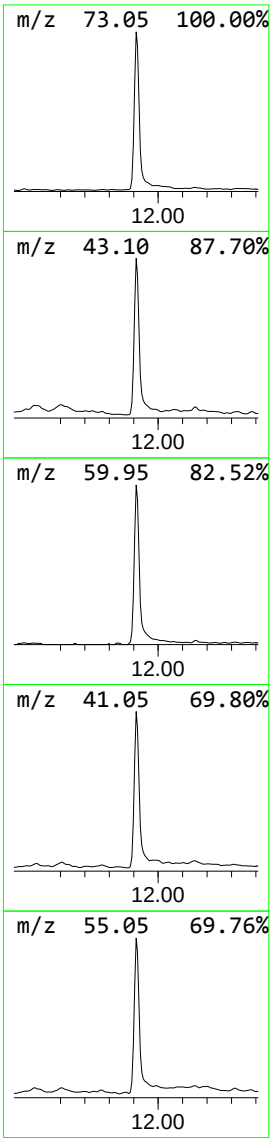
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	12.26 ng	488196	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

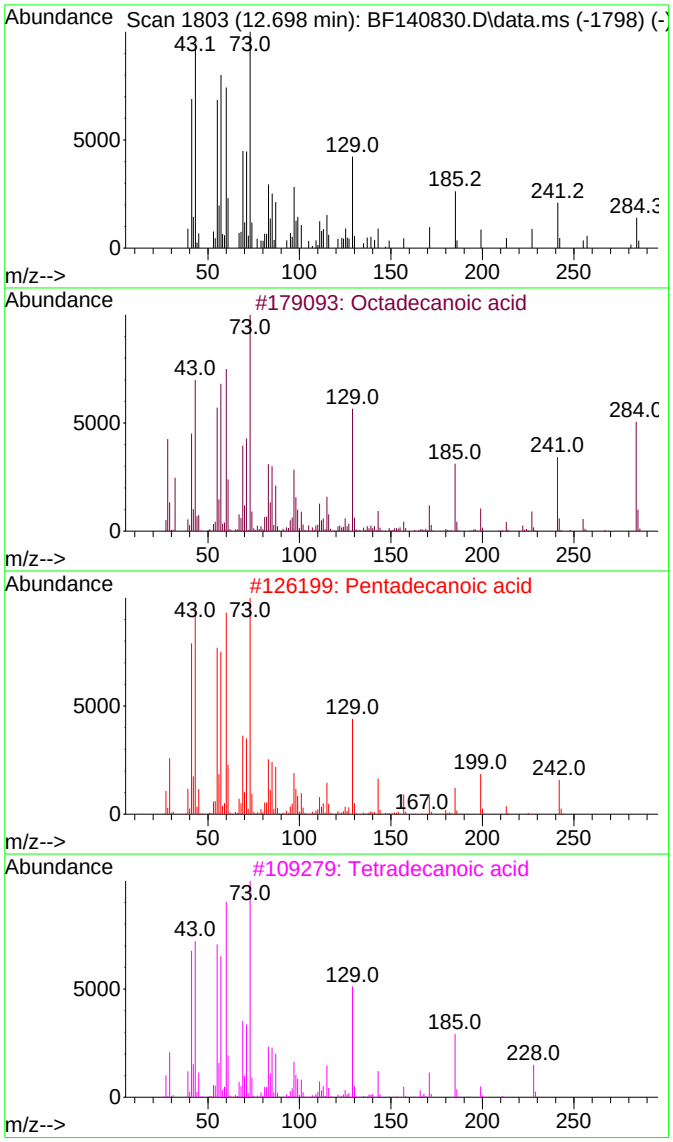
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

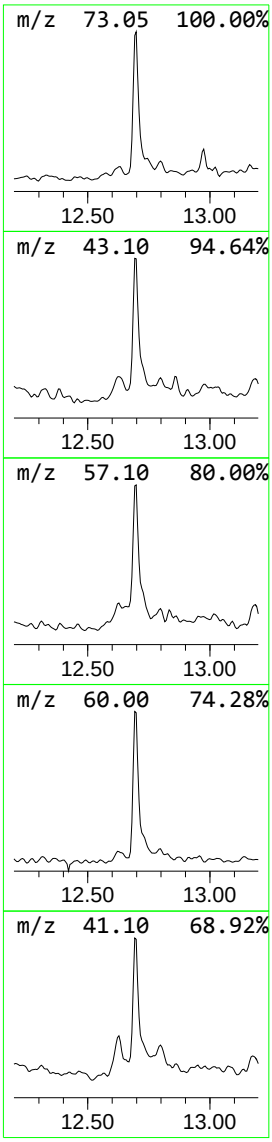
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.84 ng	112935	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

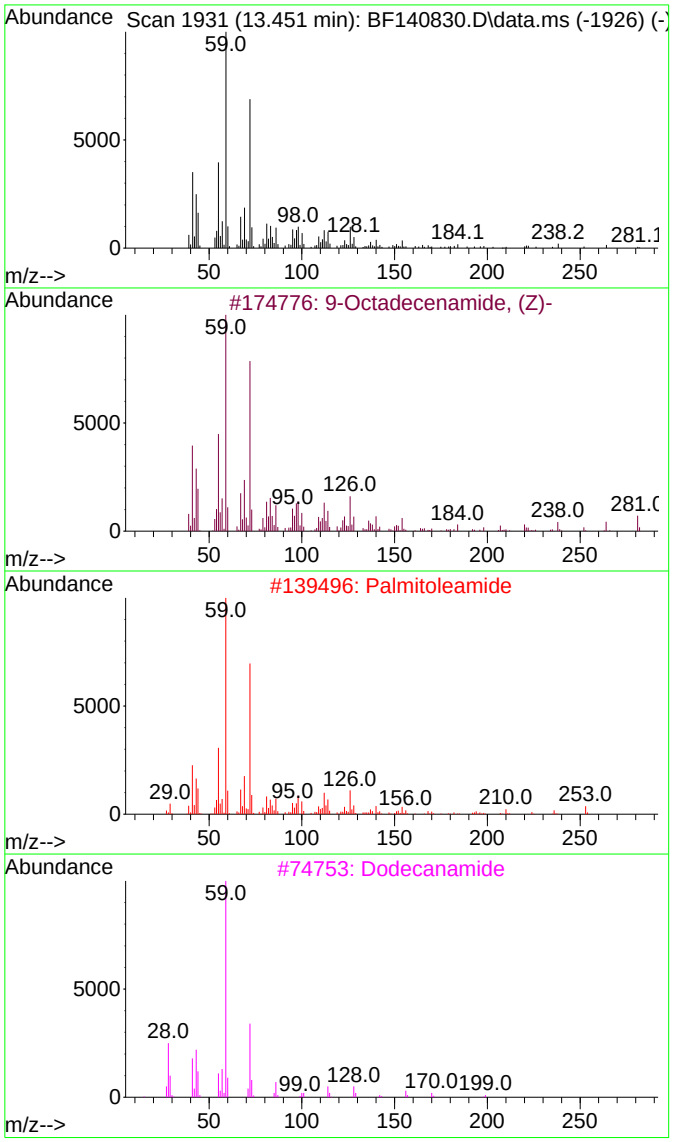
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

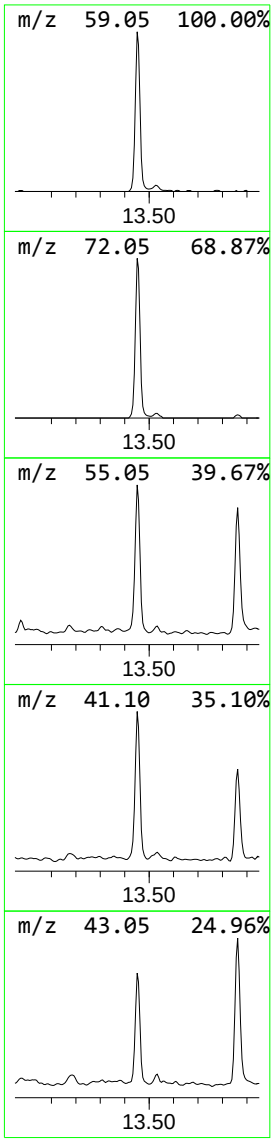
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	9.79 ng	227462	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Octanamide	143	C8H17NO	000629-01-6	59
5	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

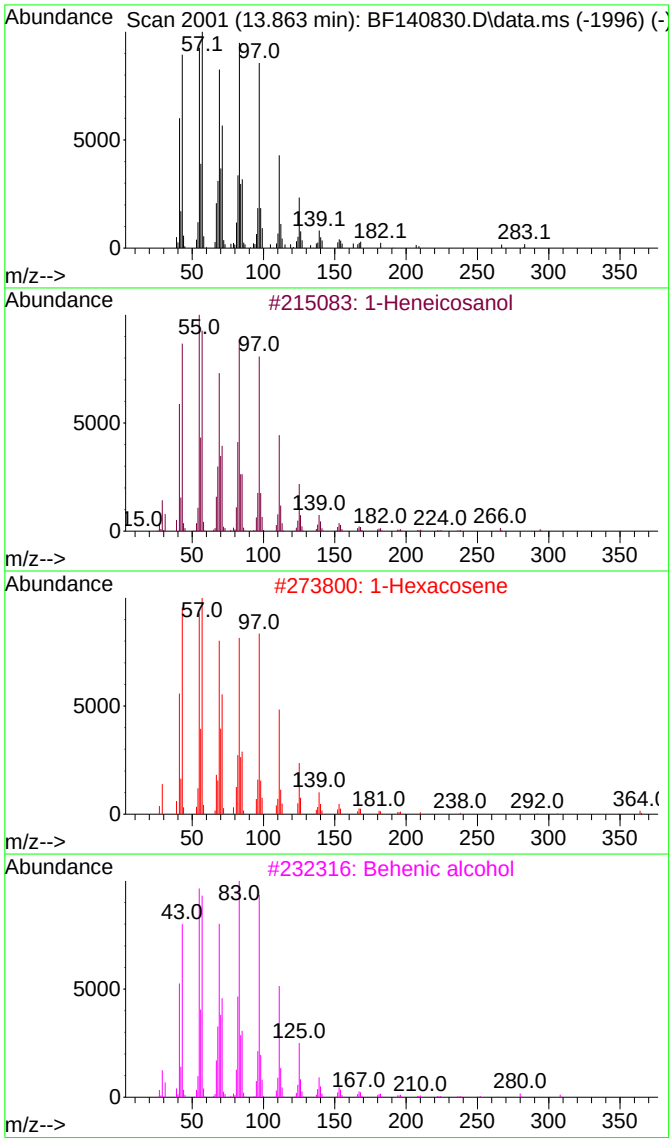
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

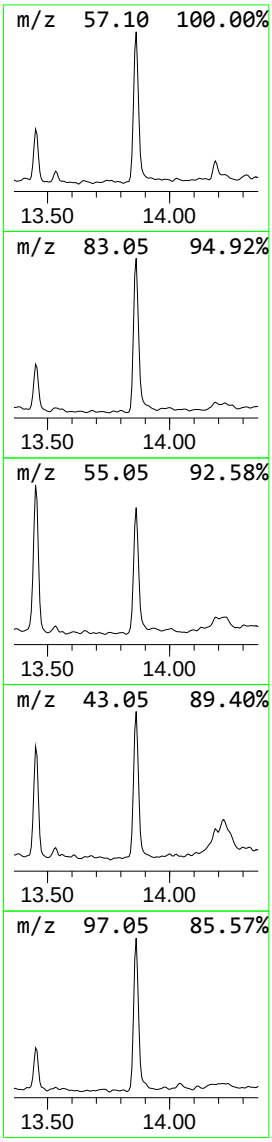
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	7.22 ng	167837	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	1-Tetracosene	336	C24H48	010192-32-2	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

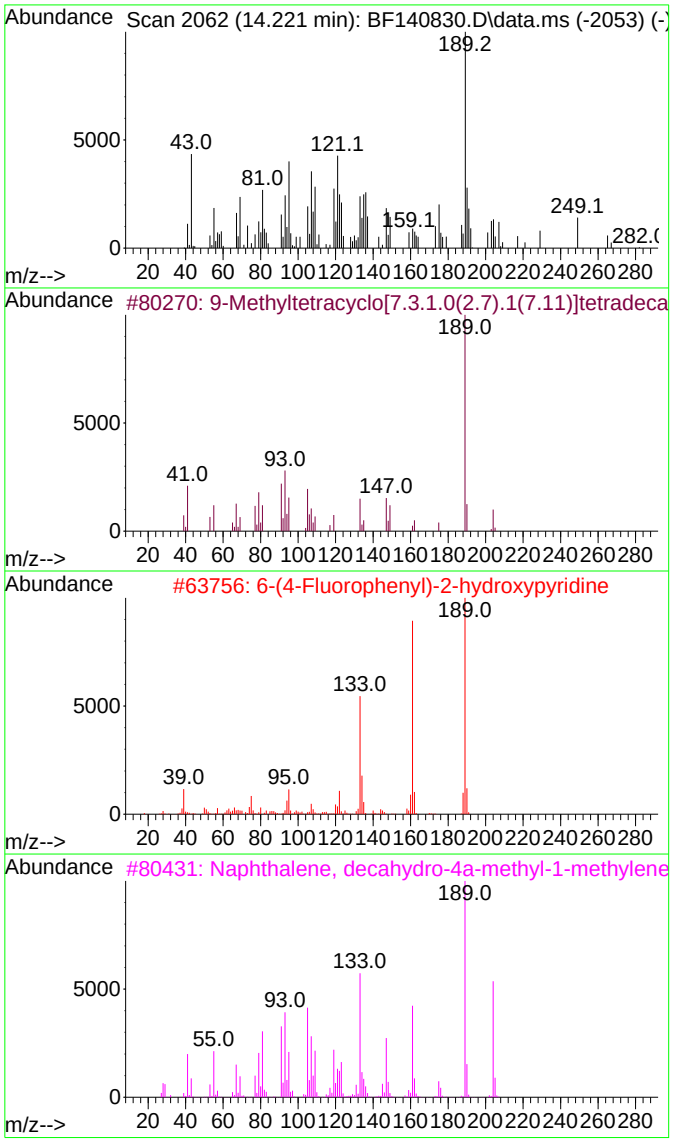
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

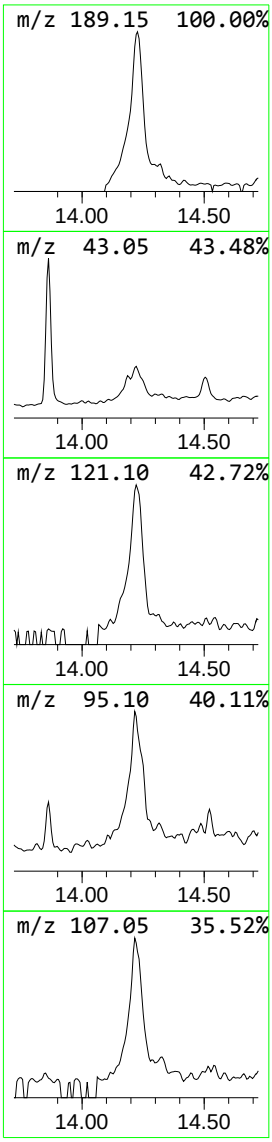
****

Peak Number 7 unknown14.221 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	4.65 ng	108033	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methyltetracyclo[7.3.1.0(2.7)....	204	C15H24	1000215-30-5	46
2	6-(4-Fluorophenyl)-2-hydroxypyri...	189	C11H8FNO	1010509-20-5	46
3	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	32
4	Naphthalene, 2,3,4,4a,5,6-hexahy...	204	C15H24	000473-14-3	32
5	(3S,3aR,6R,8aS)-7,7-Dimethyl-8-m...	218	C15H22O	082509-29-3	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140830.D
Acq On : 11 Dec 2024 15:42
Operator : RC/JU
Sample : P5216-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-744

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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...	2.140	95.3	ng	2335860	1	6.857	490408	20.0
Benzophenone	10.610	4.2	ng	163065	3	9.898	774474	20.0
n-Hexadecanoic ...	11.910	12.3	ng	488196	4	11.392	796536	20.0
Octadecanoic acid	12.698	2.8	ng	112935	4	11.392	796536	20.0
9-Octadecenamid...	13.451	9.8	ng	227462	5	14.045	464637	20.0
1-Heneicosanol	13.863	7.2	ng	167837	5	14.045	464637	20.0
unknown14.221	14.221	4.7	ng	108033	5	14.045	464637	20.0