LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	14	rVB	385055	484594	7.75%	1.757%
2	5.081	504	509	517	rVB	605935	770593	12.32%	2.794%
3	5.487	573	578	581	rBV	1917858	1800372	28.78%	6.528%
4	6.504	746	751	754	rBV	1869863	1743126	27.86%	6.320%
5	6.875	810	814	817	rBV	530058	431767	6.90%	1.565%
6	7.440	905	910	913	rBV	1233310	1147200	18.34%	4.159%
7	8.163	1029	1033	1036	rBV	652572	497563	7.95%	1.804%
8	9.239	1212	1216	1220	rBV	1983000	1776390	28.40%	6.441%
9	9.922	1329	1332	1336	rVB	622471	496601	7.94%	1.801%
10	10.716	1463	1467	1470	rBV	1157940	928001	14.83%	3.365%
11	11.416	1582	1586	1588	rBV	533261	439431	7.02%	1.593%
12	11.439	1588	1590	1594	rVB	219538	170820	2.73%	0.619%
13	11.810	1649	1653	1656	rBV	1155223	968504	15.48%	3.512%
14	11.945	1673	1676	1680	rVB	168946	134717	2.15%	0.488%
15	12.510	1767	1772	1773	rBV	5797765	6255734	100.00%	22.682%
16	12.527	1773	1775	1781	rVV2	4980337	4077786	65.18%	14.785%
17	12.604	1785	1788	1791	rBV	889227	731715	11.70%	2.653%
18	12.639	1791	1794	1797	rBV2	446473	580840	9.28%	2.106%
19	12.663	1797	1798	1808	rVB4	210854	195278	3.12%	0.708%
20	12.869	1826	1833	1838	rBV	318693	327702	5.24%	1.188%
21	13.010	1853	1857	1861	rVB	1399318	1184519	18.93%	4.295%
22	13.198	1886	1889	1892	rVB	60595	66841	1.07%	0.242%
23	13.257	1897	1899	1903	rVB2	68611	75375	1.20%	0.273%
24	13.333	1909	1912	1914	rBV2	91594	74061	1.18%	0.269%
25	13.916	2007	2011	2020	rVB4	109856	174532	2.79%	0.633%
26	14.004	2023	2026	2029	rVB	101505	87090	1.39%	0.316%
27	14.069	2030	2037	2040	rBV2	572462	695328	11.12%	2.521%
28	14.098	2040	2042	2048	rVB	156958	149931	2.40%	0.544%
29	14.927	2180	2183	2187	rBV	70168	69807	1.12%	0.253%
30	15.127	2213	2217	2220	rBV	133423	198788	3.18%	0.721%
31	15.439	2266	2270	2276	rVB	79338	105002	1.68%	0.381%
32	15.504	2277	2281	2287	rBV	119047	159958	2.56%	0.580%
33	15.574	2288	2293	2297	rBV	367974	490473	7.84%	1.778%
34	17.080	2545	2549	2559	rVB4	40878	90114	1.44%	0.327%

Sum of corrected areas: 27580553

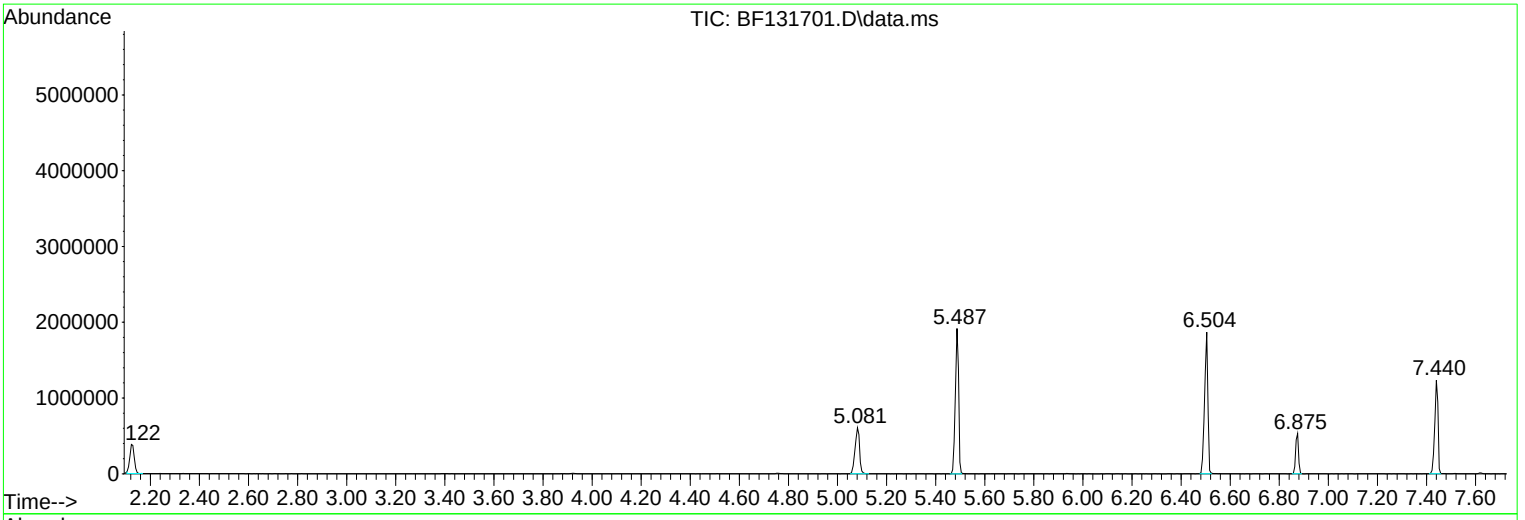
Instrument :
BNA_F
ClientSampleId :
BU-03-121522

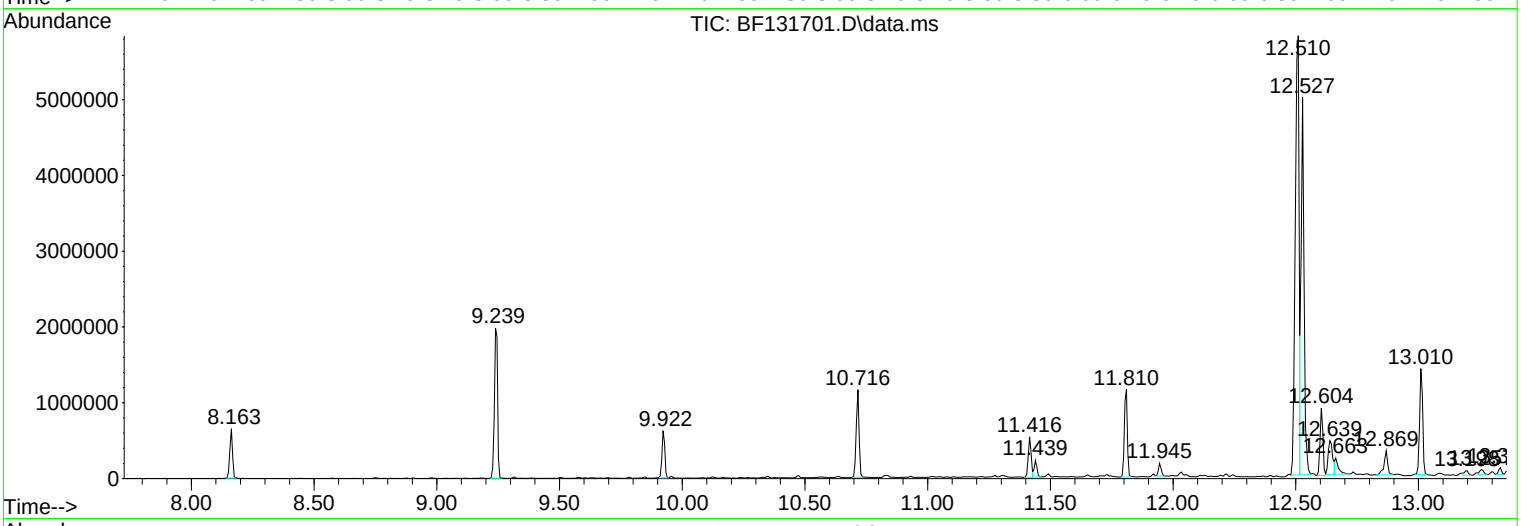
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

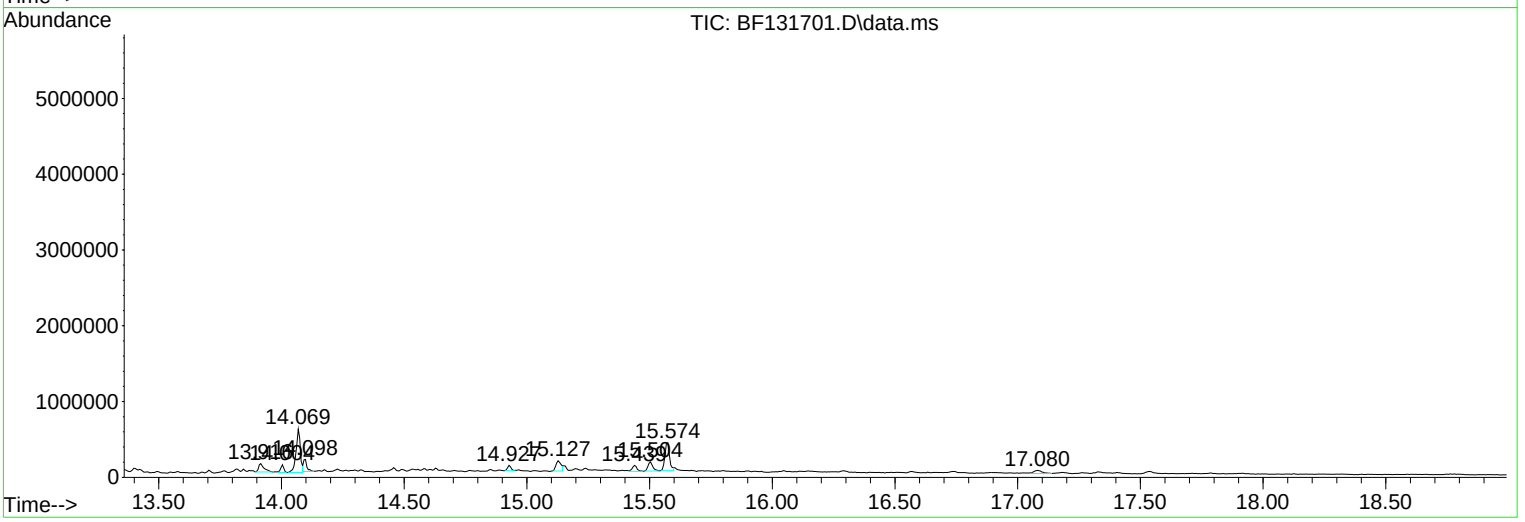
Instrument :
BNA_F
ClientSampleId :
BU-03-121522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

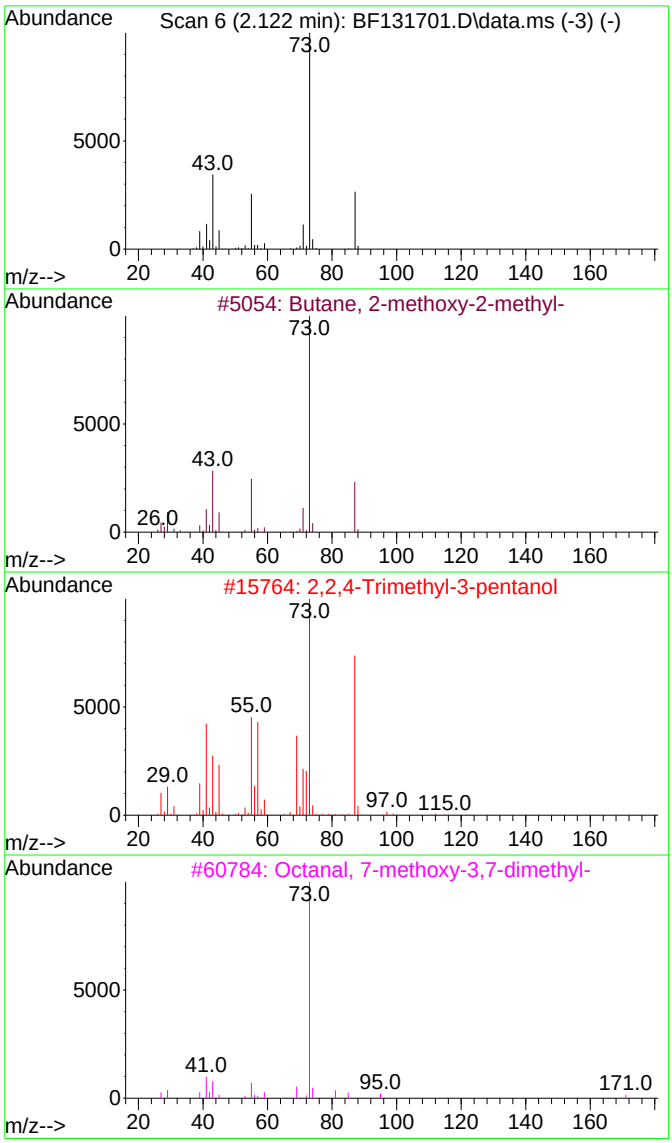
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

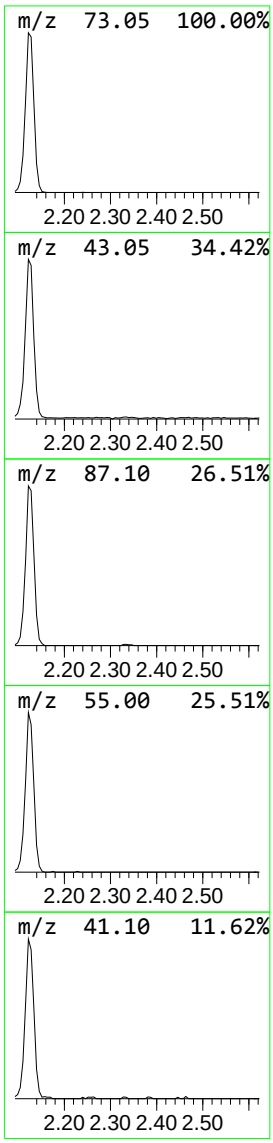
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	22.45 ng	484594	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

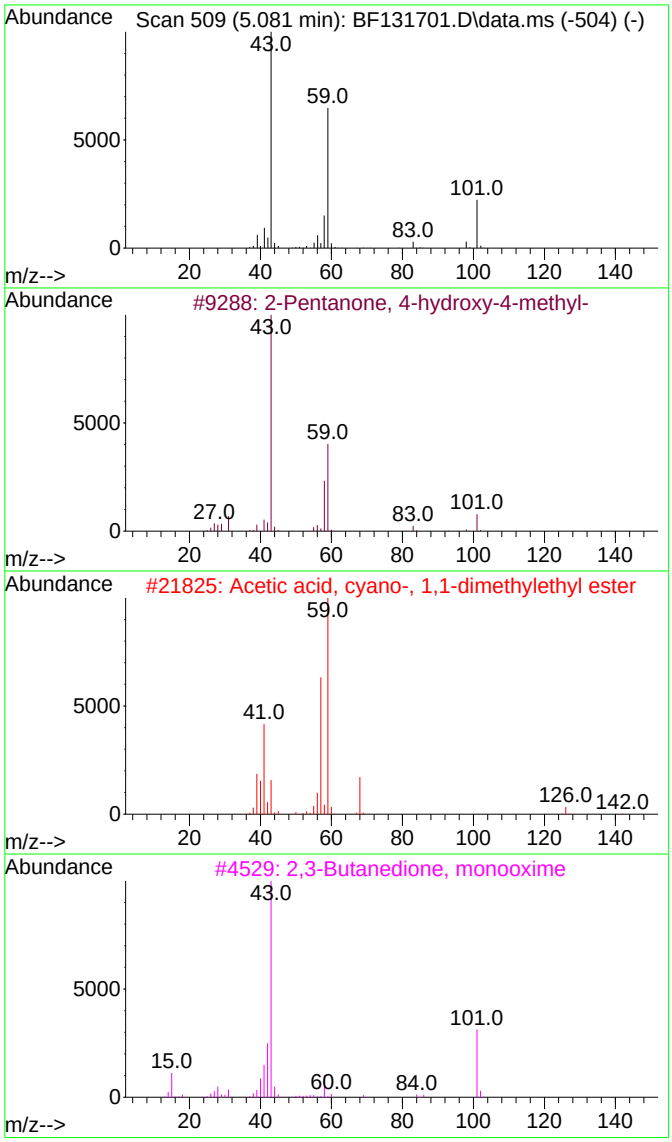
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

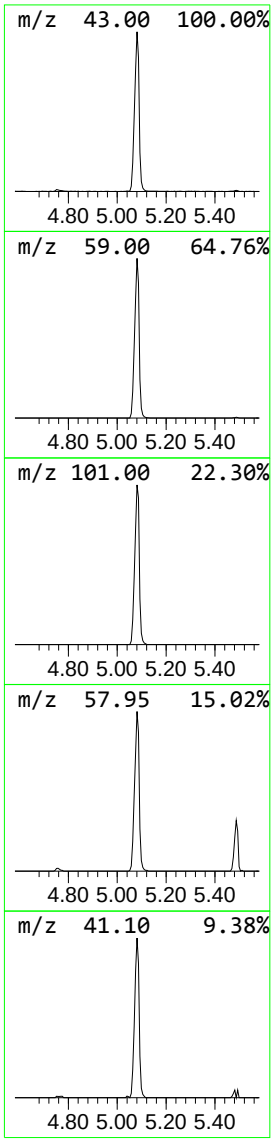
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	35.69 ng	770593	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

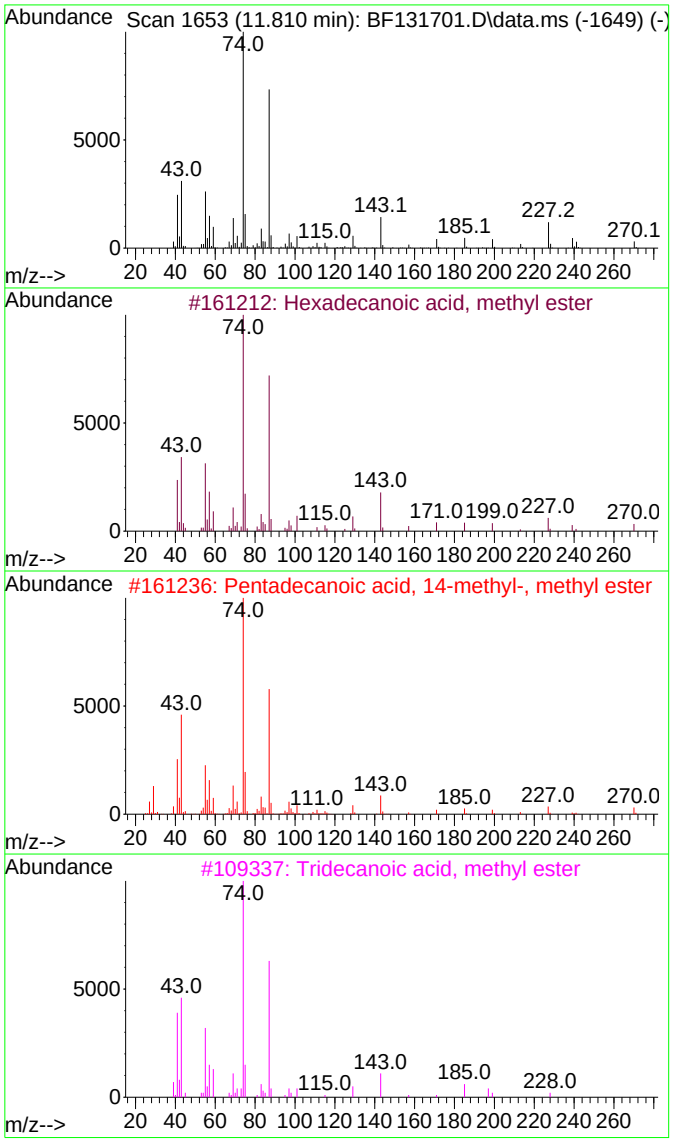
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

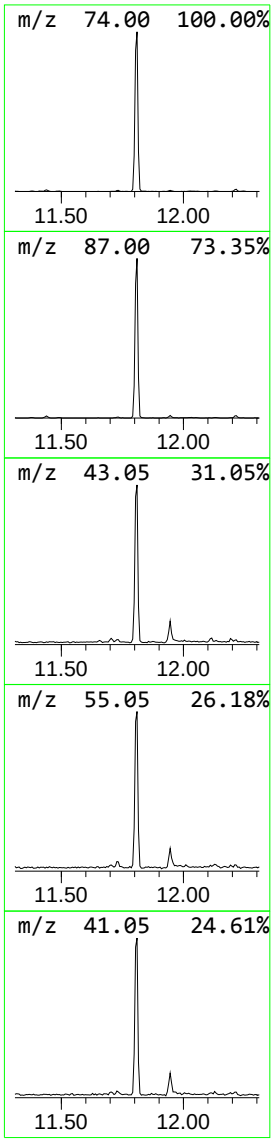
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	44.08 ng	968504	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

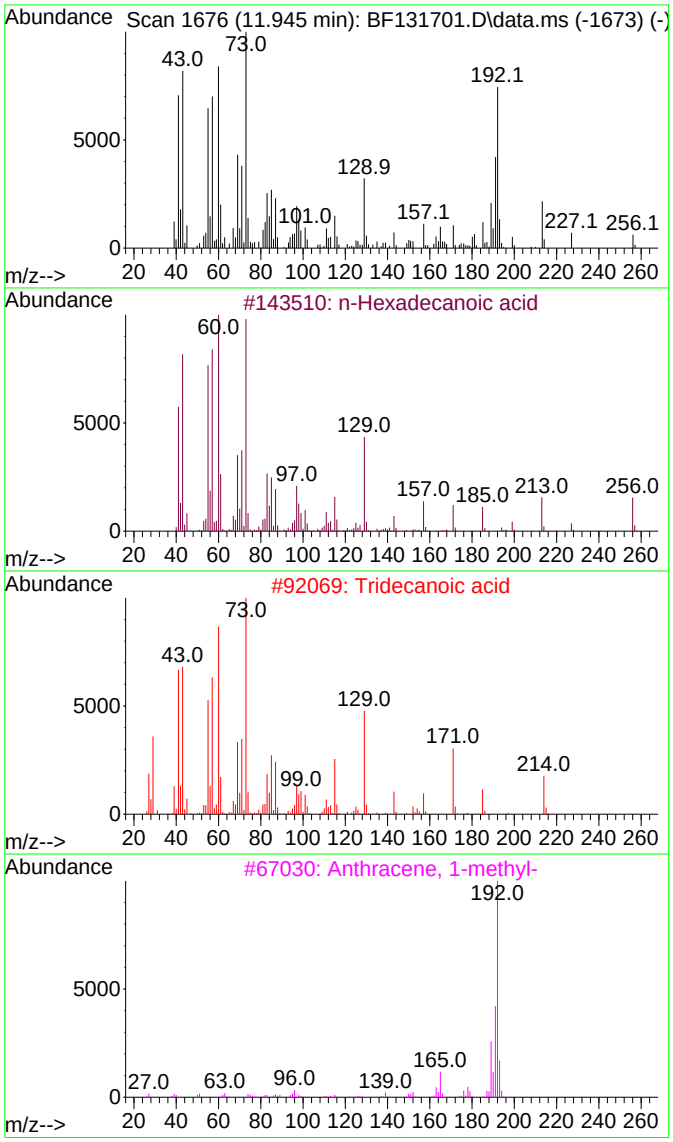
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

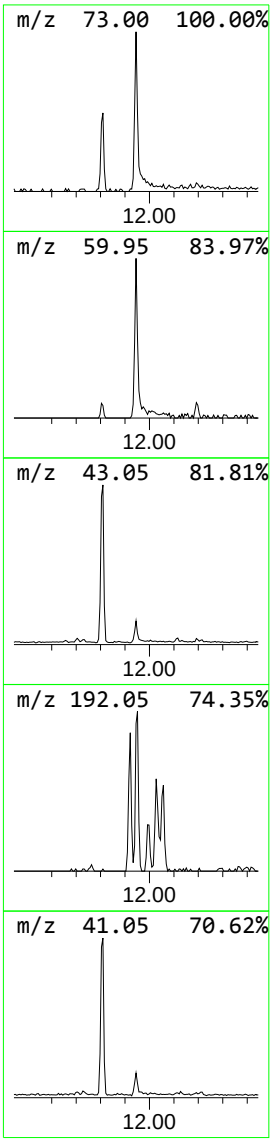
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	6.13 ng	134717	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

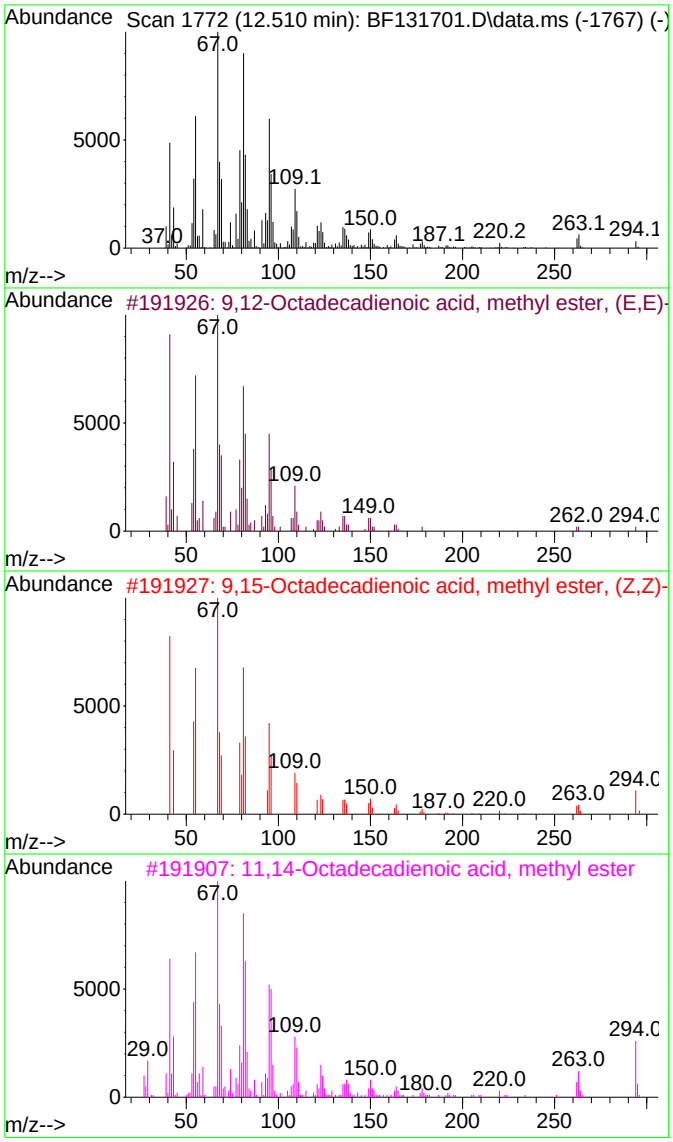
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

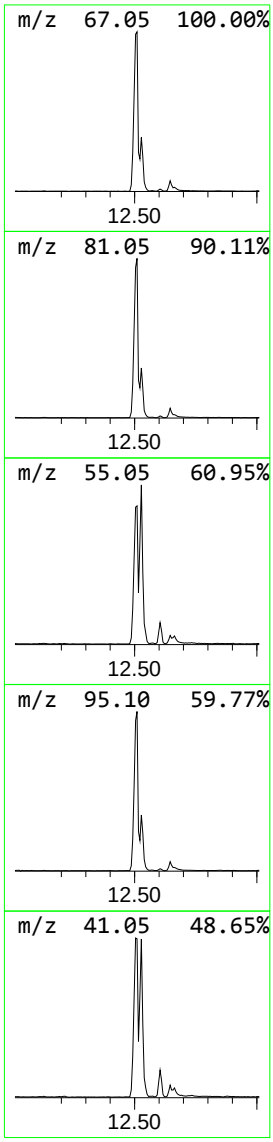
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	284.72 ng	6255730	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
3	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	97
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	96
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
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Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

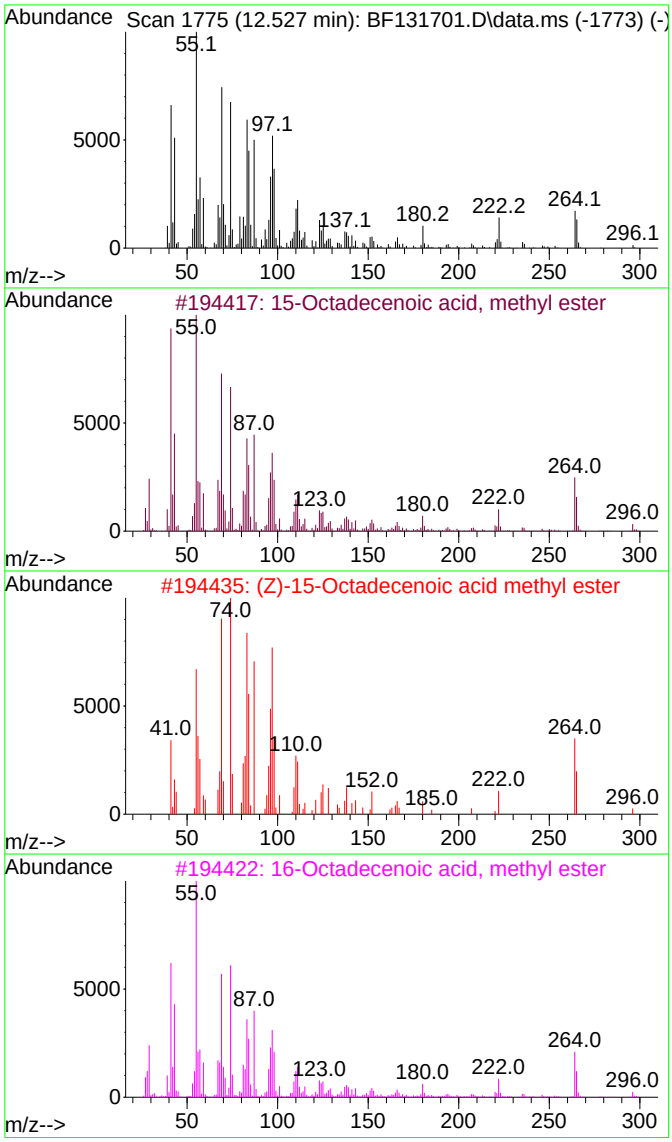
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

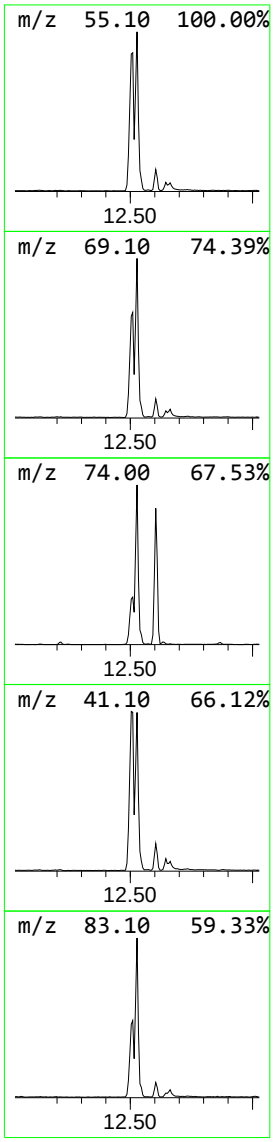
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 15-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.528	185.59 ng	4077790	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	96
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	89
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

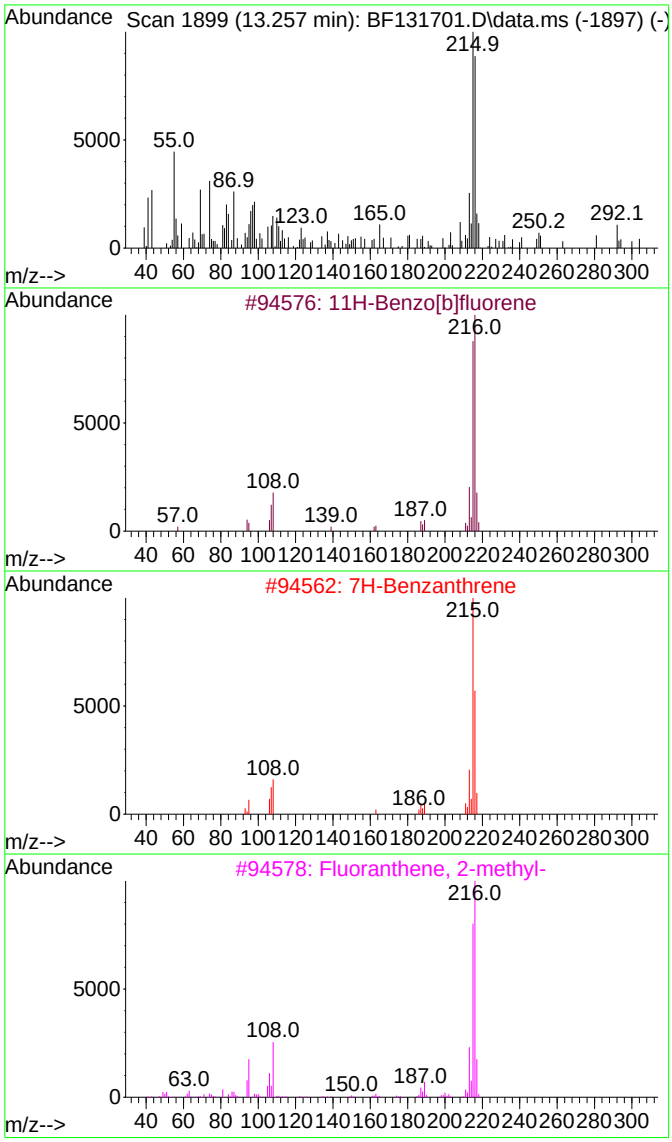
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

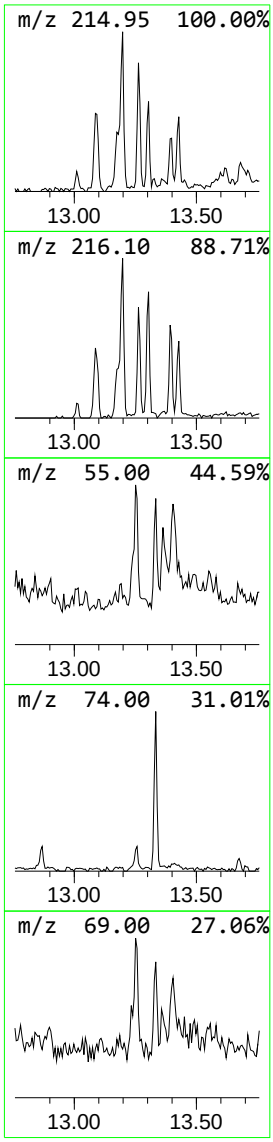
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.257	2.17 ng	75375	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	7H-Benzanthrene	216	C17H12	000199-94-0	58
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	53
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	50
5	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
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Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

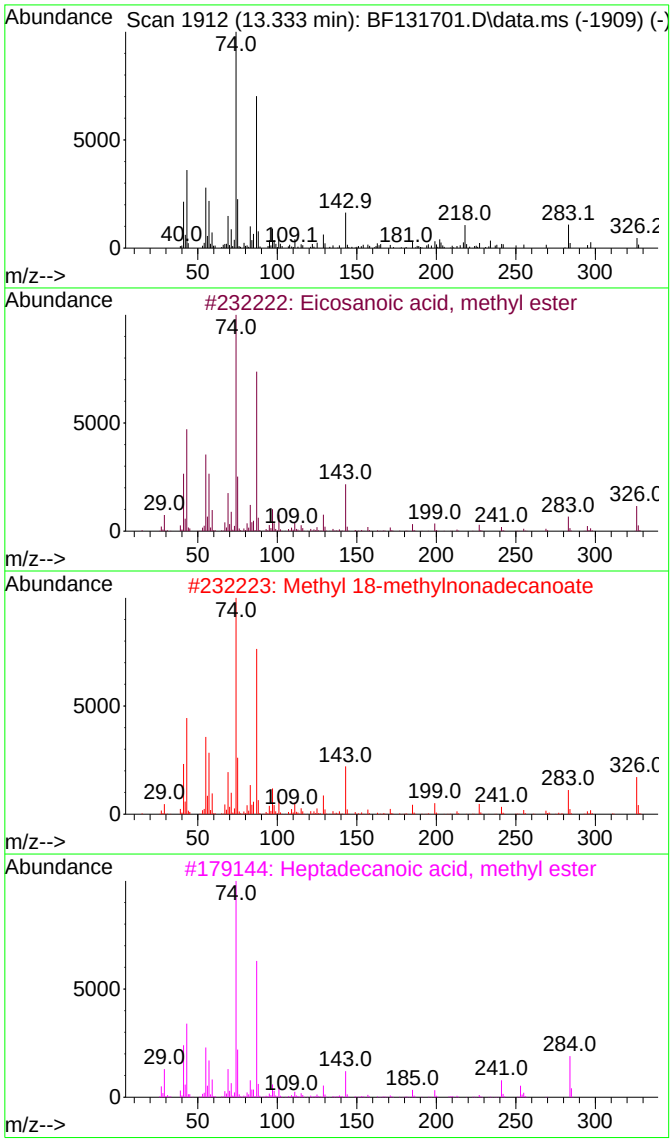
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

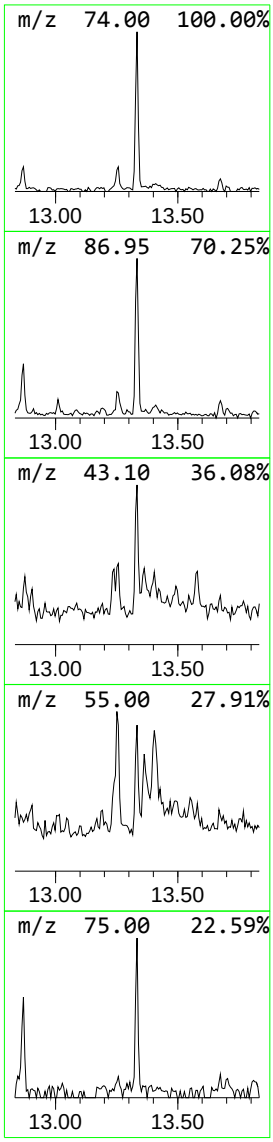
****

Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	2.13 ng	74061	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	97
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

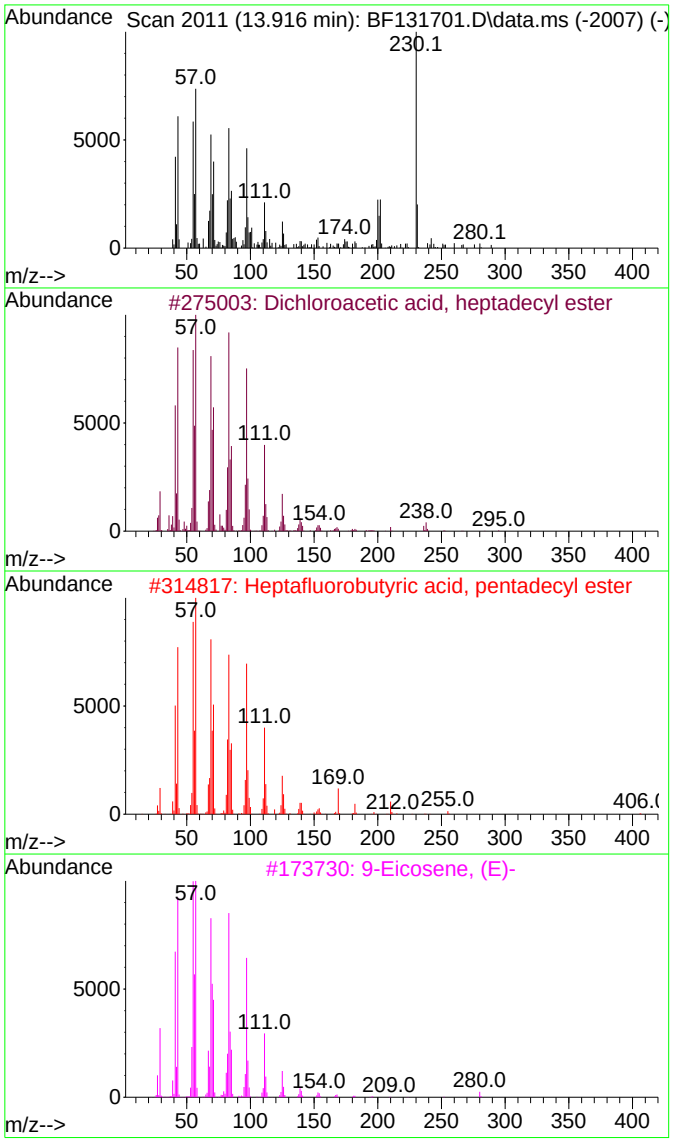
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

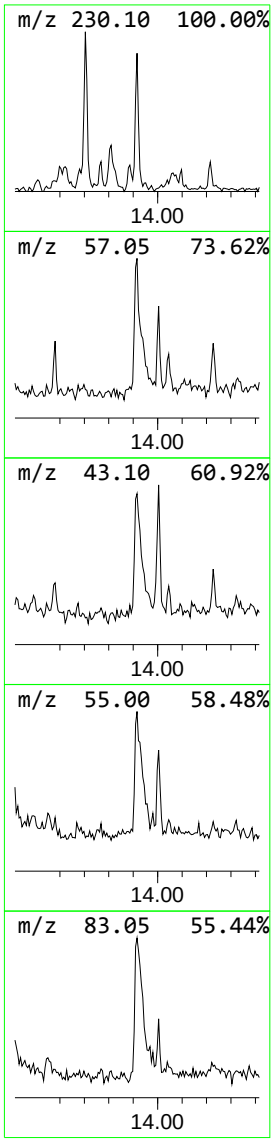
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	5.02 ng	174532	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	70
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	64
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	62
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	60
5	1-Octadecene	252	C18H36	000112-88-9	59





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Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

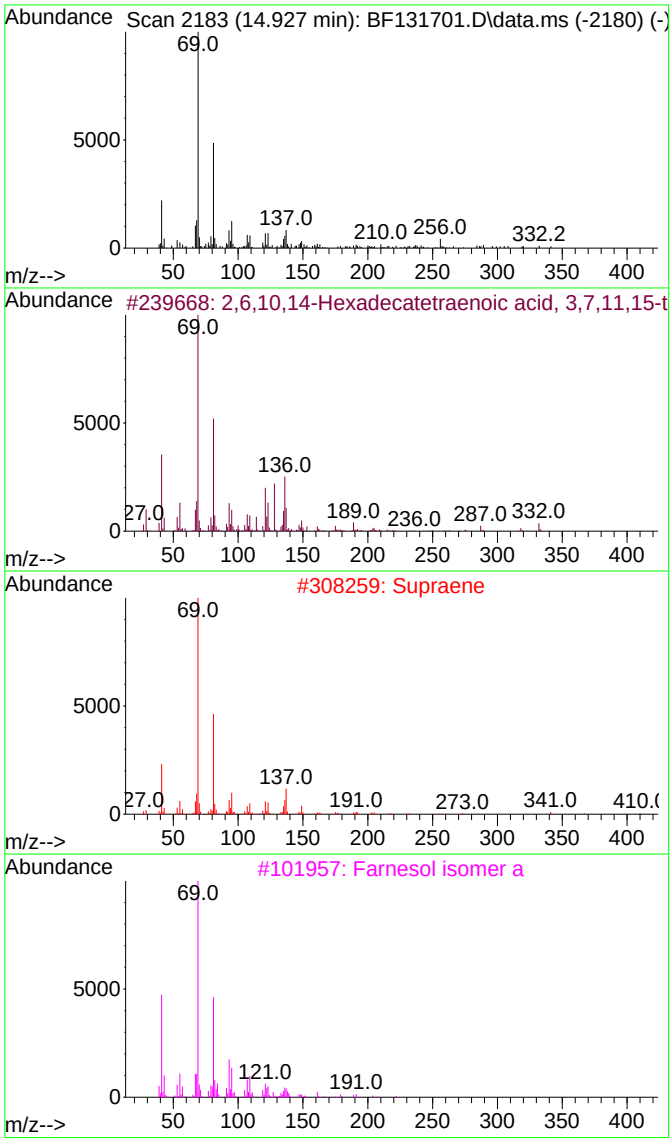
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

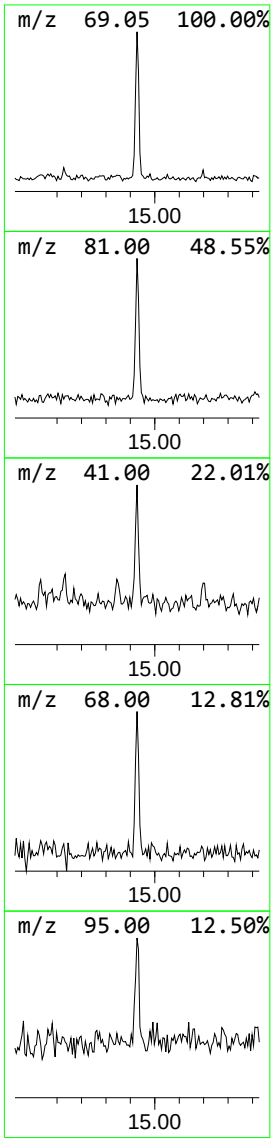
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,6,10,14-Hexadecatetraenoi... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	2.85 ng	69807	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	74
2	Supraene	410	C30H50	007683-64-9	74
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	Squalene	410	C30H50	000111-02-4	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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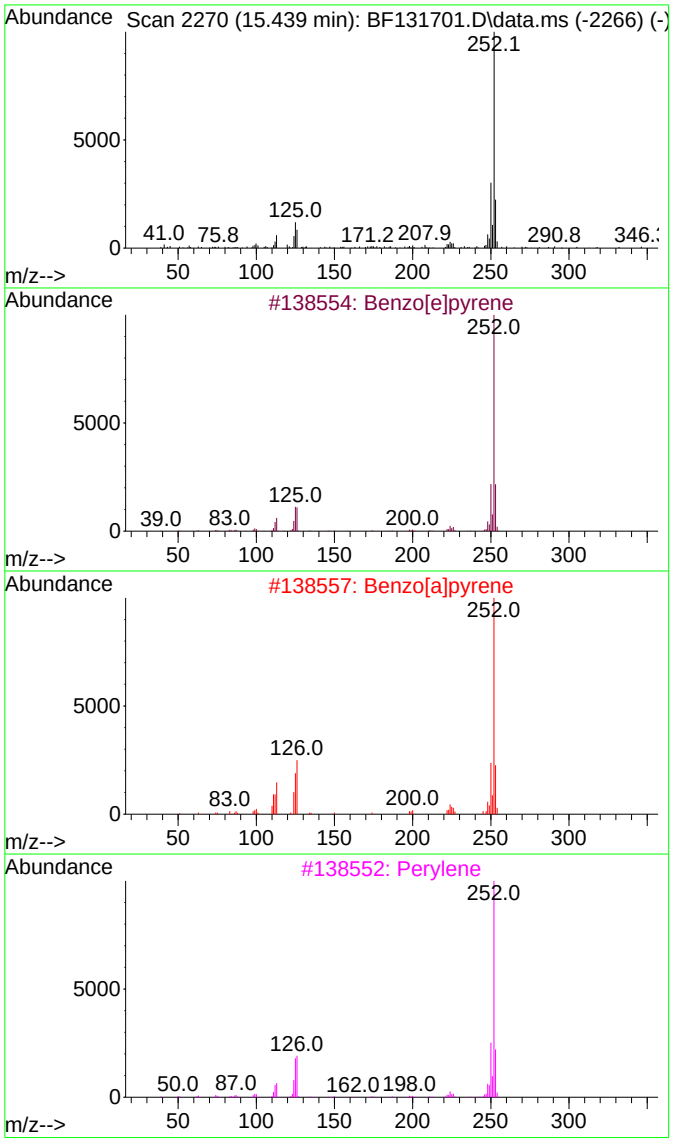
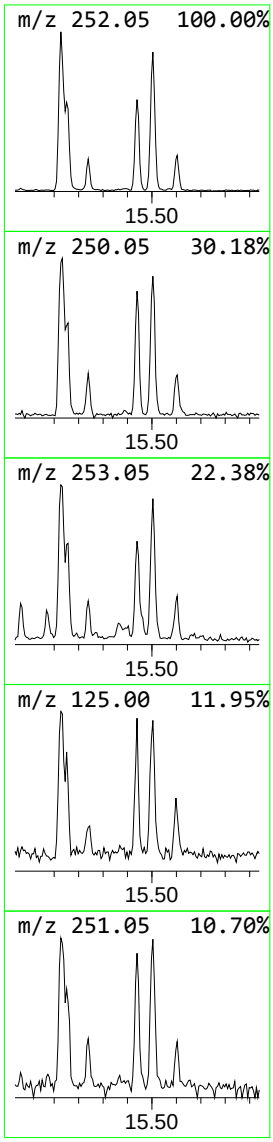
Peak Number 11 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	4.28 ng	105002	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131701.D
Acq On : 19 Dec 2022 21:44
Operator : CG\JU
Sample : N6091-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-121522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.122	22.4	ng	484594	1	6.875	431767	20.0
2-Pentanone, 4-...	5.081	35.7	ng	770593	1	6.875	431767	20.0
Hexadecanoic ac...	11.810	44.1	ng	968504	4	11.416	439431	20.0
n-Hexadecanoic ...	11.945	6.1	ng	134717	4	11.416	439431	20.0
9,12-Octadecadi...	12.510	284.7	ng	6255730	4	11.416	439431	20.0
15-Octadecenoic...	12.528	185.6	ng	4077790	4	11.416	439431	20.0
11H-Benzo[b]flu...	13.257	2.2	ng	75375	5	14.069	695328	20.0
Eicosanoic acid...	13.333	2.1	ng	74061	5	14.069	695328	20.0
Dichloroacetic ...	13.916	5.0	ng	174532	5	14.069	695328	20.0
2,6,10,14-Hexad...	14.927	2.9	ng	69807	6	15.574	490473	20.0
Benzo[e]pyrene	15.439	4.3	ng	105002	6	15.574	490473	20.0