LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127770.D
Acq On : 12 Apr 2022 20:59
Operator : CG\JU
Sample : N2333-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127770.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	13	19	31	rVB3	78552	129349	2.89%	0.569%
2	3.881	266	271	278	rBV	53490	68090	1.52%	0.299%
3	4.551	381	385	396	rBV2	114326	140785	3.14%	0.619%
4	4.981	450	458	466	rBV2	88215	105851	2.36%	0.465%
5	5.181	488	492	497	rVB	96292	100775	2.25%	0.443%
6	5.575	554	559	562	rBV	1830872	1607878	35.88%	7.069%
7	6.569	724	728	731	rBV	1240564	981213	21.89%	4.314%
8	6.957	790	794	797	rBV	931515	772906	17.25%	3.398%
9	7.522	884	890	893	rBV	2619870	2522767	56.29%	11.092%
10	8.239	1008	1012	1015	rBV	1142312	931030	20.77%	4.093%
11	8.816	1107	1110	1115	rVB2	54806	56230	1.25%	0.247%
12	9.316	1190	1195	1198	rBV	5066988	4481497	100.00%	19.703%
13	9.998	1307	1311	1314	rVB	1214952	1033545	23.06%	4.544%
14	10.369	1371	1374	1377	rBV	95207	73606	1.64%	0.324%
15	10.786	1441	1445	1448	rBV	2972962	2736204	61.06%	12.030%
16	11.486	1560	1564	1568	rBV	1181493	978392	21.83%	4.302%
17	12.004	1649	1652	1657	rBV	121917	130748	2.92%	0.575%
18	13.080	1830	1835	1838	rBV	3690135	3672951	81.96%	16.148%
19	13.980	1985	1988	1998	rVB2	143677	187975	4.19%	0.826%
20	14.104	2006	2009	2011	rBV	216943	178906	3.99%	0.787%
21	14.133	2011	2014	2018	rVB	967161	814430	18.17%	3.581%
22	14.763	2118	2121	2123	rBV	96396	93690	2.09%	0.412%
23	15.657	2267	2273	2279	rBV	724402	946203	21.11%	4.160%

Sum of corrected areas: 22745021

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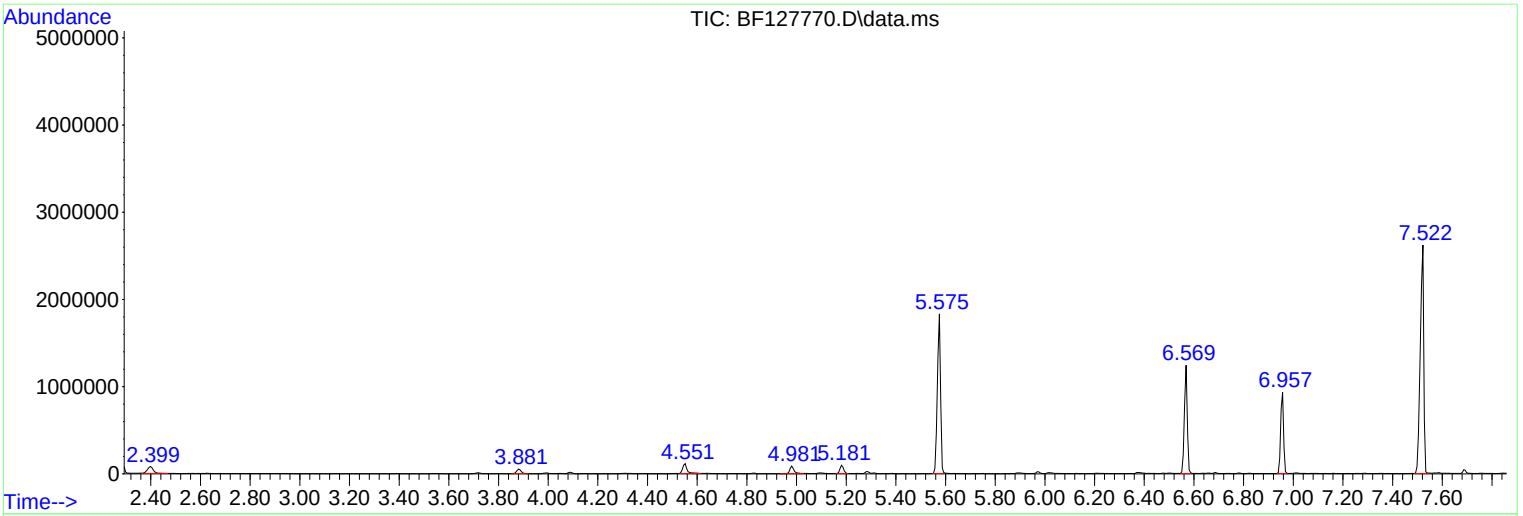
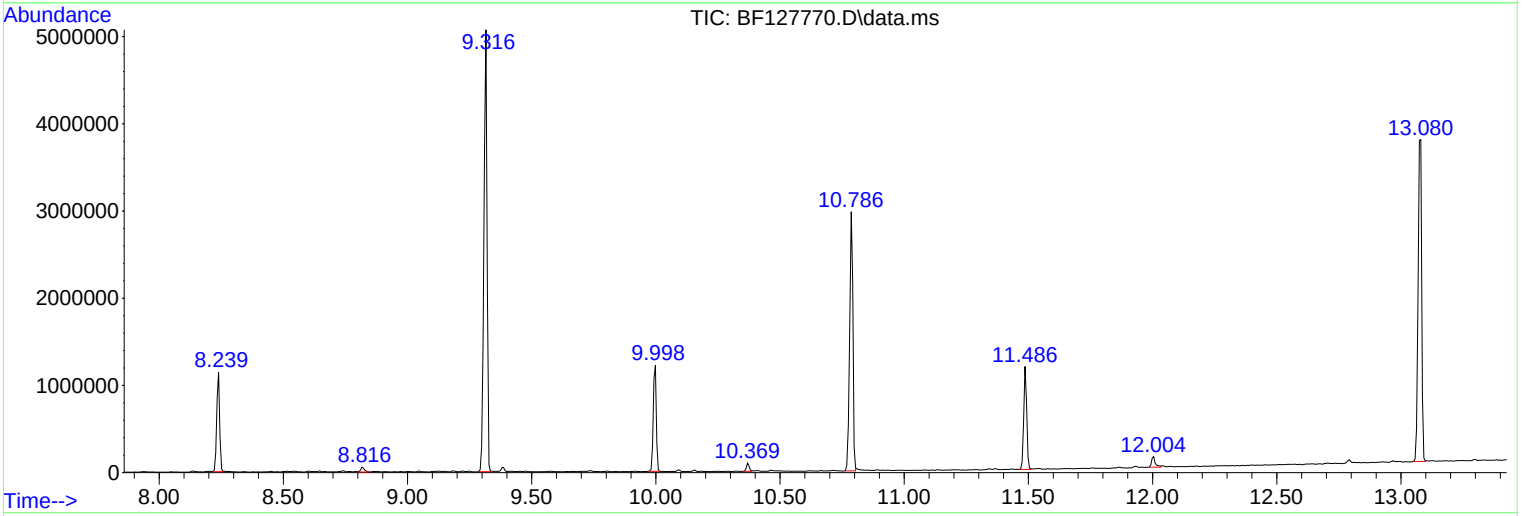
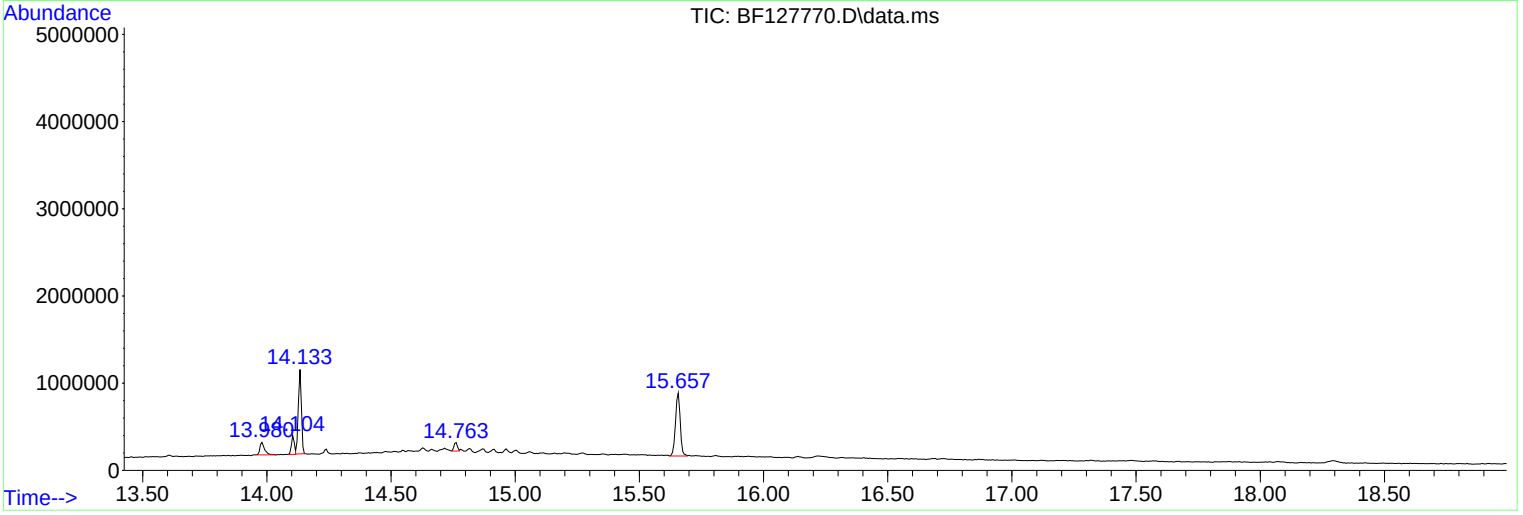
BNA_F
ClientSampleId :
MW-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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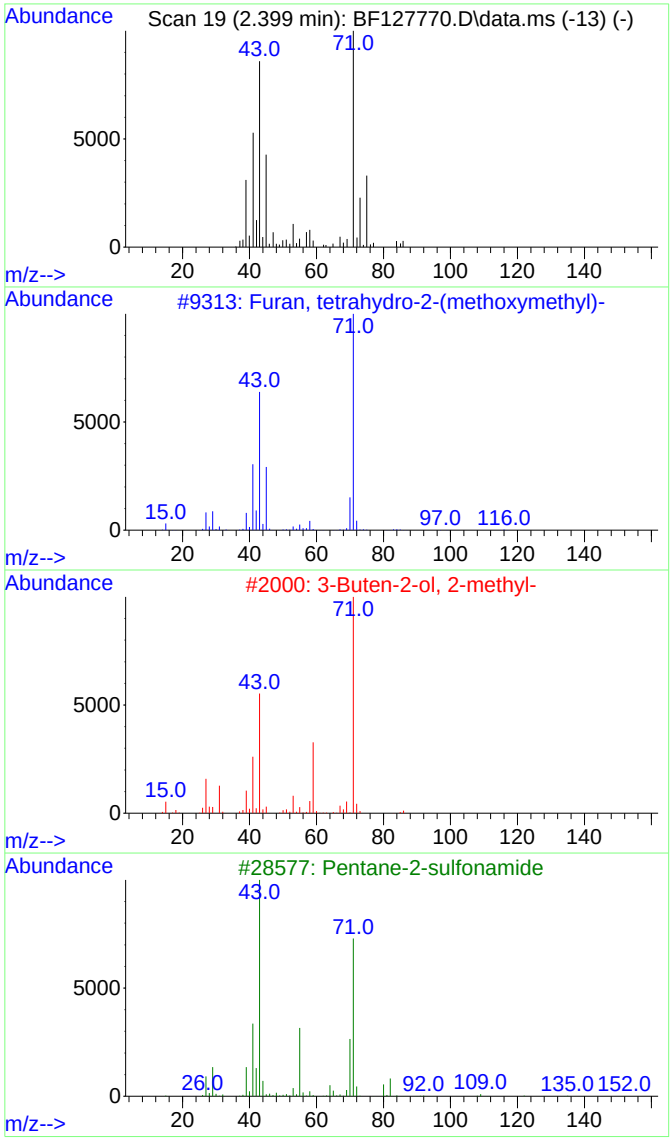
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

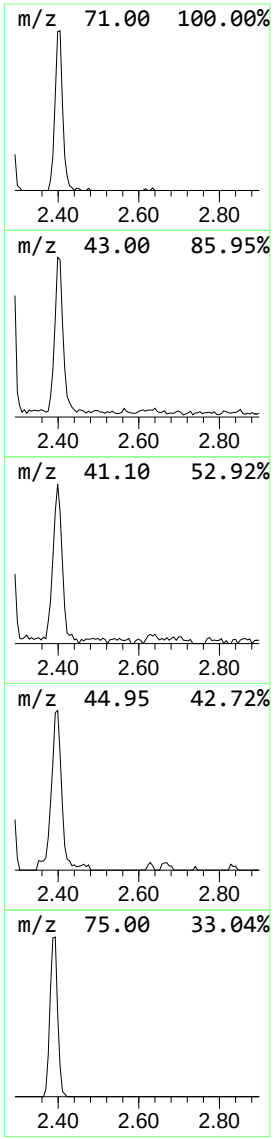
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	3.35 ng	129349	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	58
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	38
3	Pentane-2-sulfonamide	151	C5H13NO2S	017854-62-5	38
4	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38
5	Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	35





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Operator : CG\JU
Sample : N2333-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

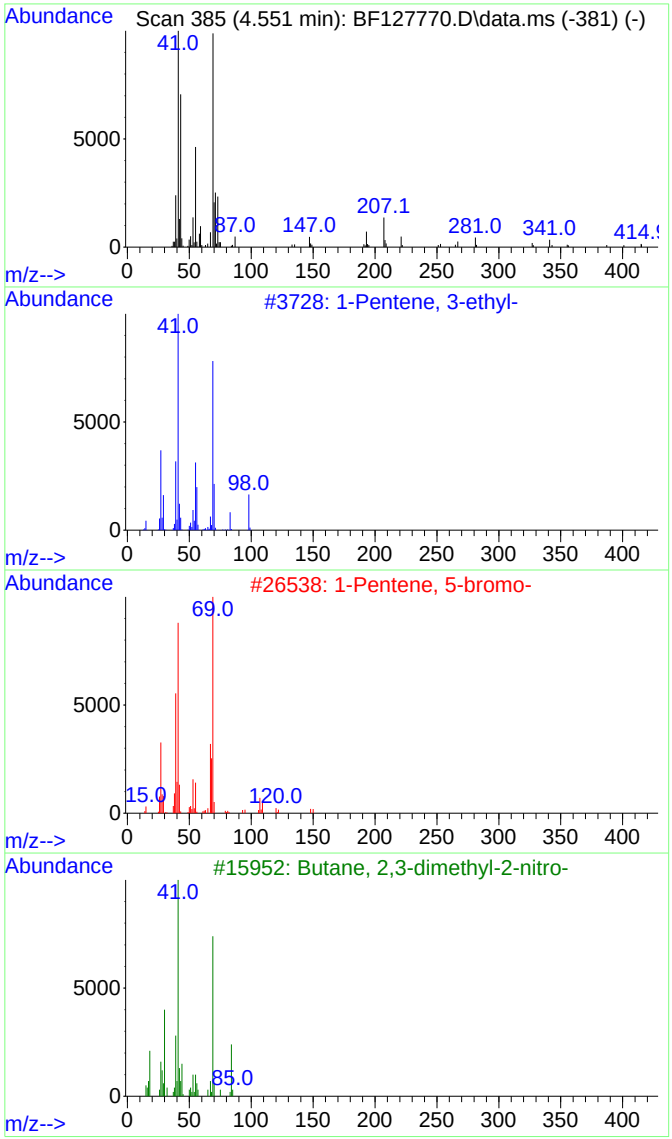
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

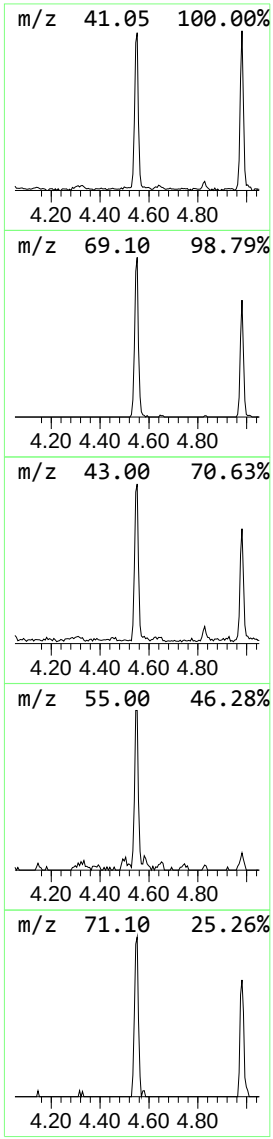
****

Peak Number 2 unknown4.551 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	3.64 ng	140785	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	43
2	1-Pentene, 5-bromo-	148	C5H9Br	001119-51-3	35
3	Butane, 2,3-dimethyl-2-nitro-	131	C6H13NO2	034075-28-0	35
4	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	32
5	3-Methyl-2-hexene	98	C7H14	017618-77-8	25





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Acq On : 12 Apr 2022 20:59
Operator : CG\JU
Sample : N2333-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

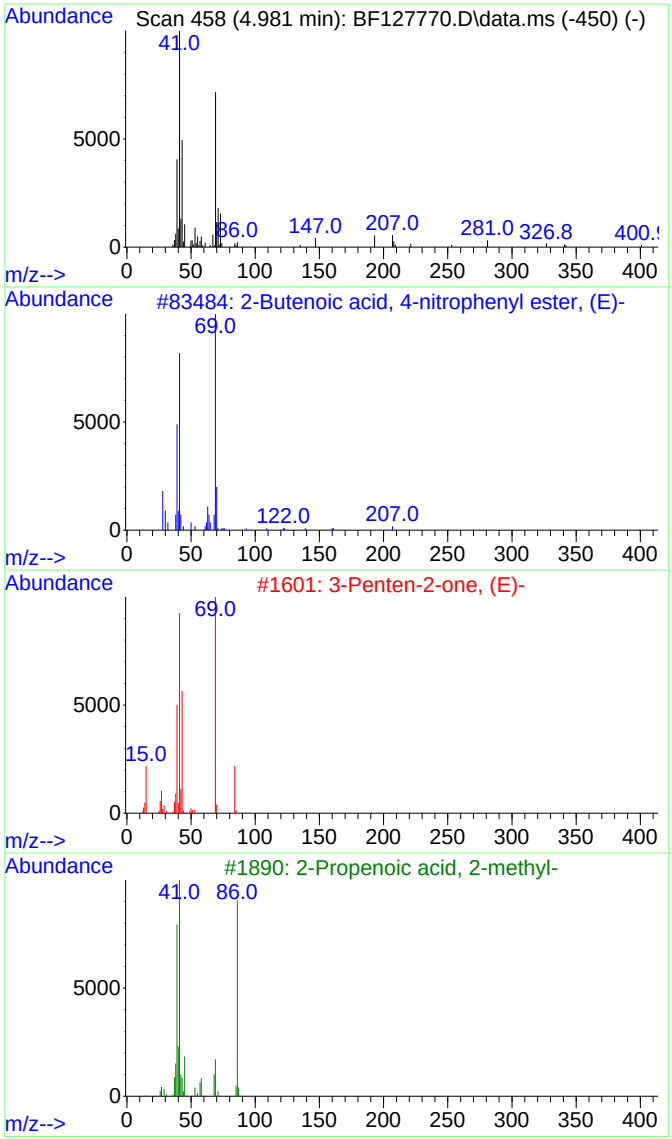
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

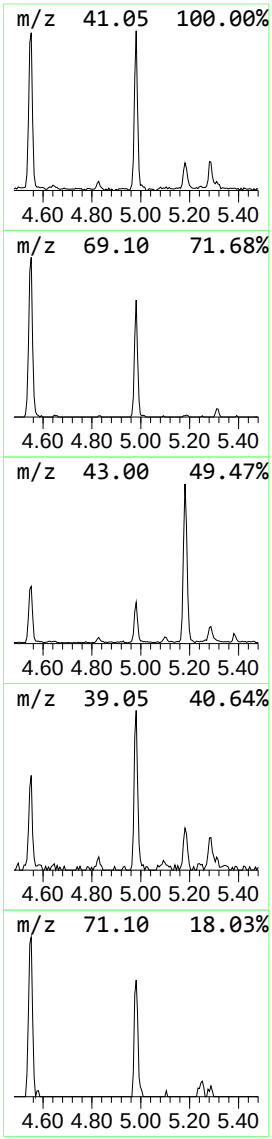
****

Peak Number 3 unknown4.981 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	2.74 ng	105851	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	43
2	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	38
3	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	32
4	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	32
5	3-Penten-2-one	84	C5H8O	000625-33-2	23





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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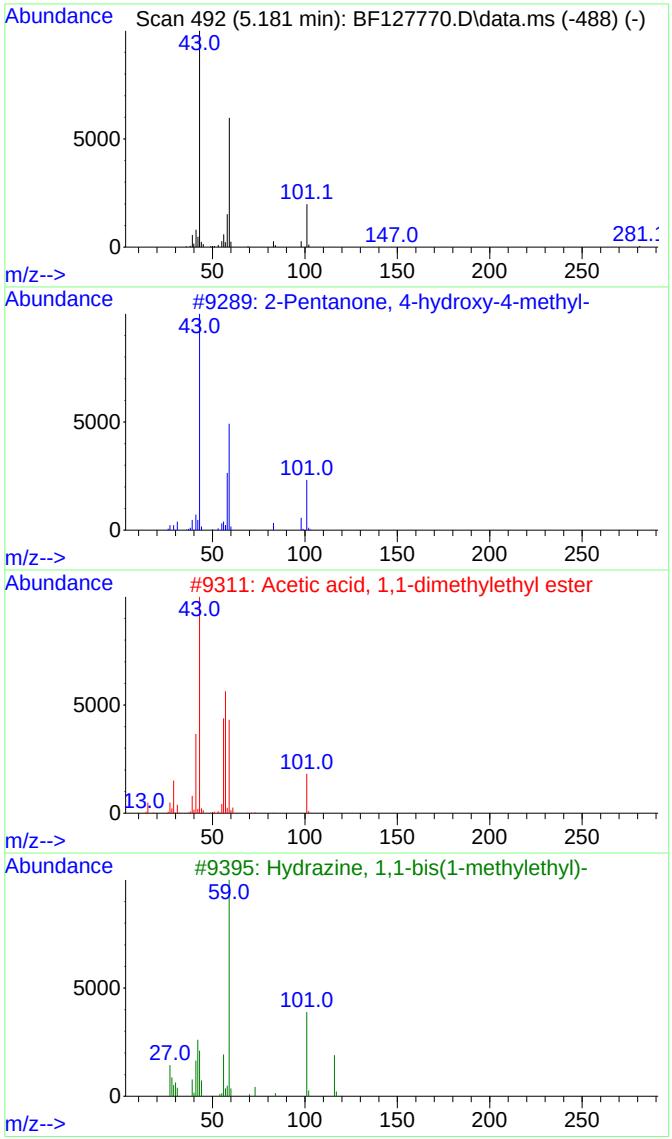
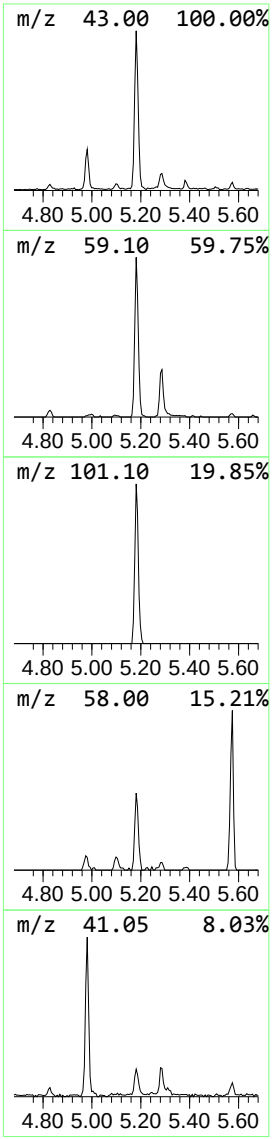
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	2.61 ng	100775	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Guanidine	59	CH5N3	000113-00-8	9





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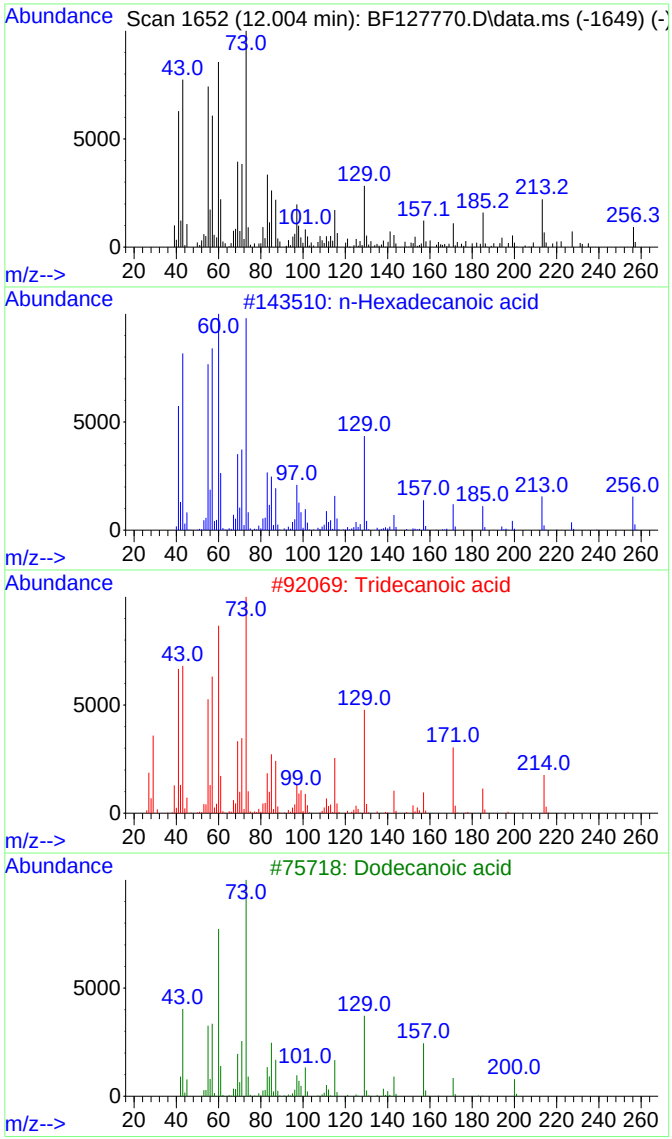
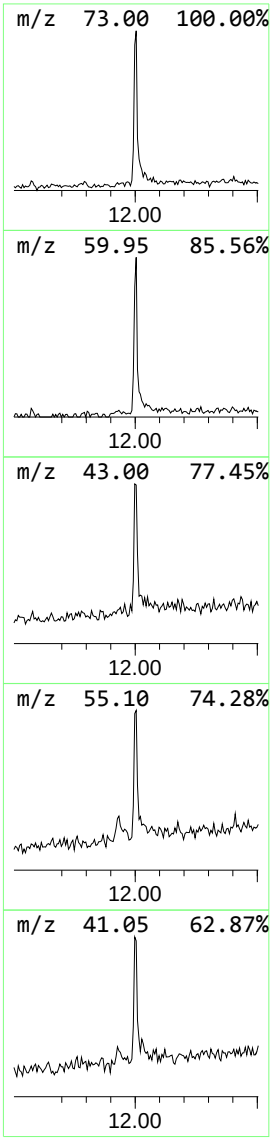
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.67 ng	130748	Phenanthrene-d10	11.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Dodecanoic acid	200	C12H24O2	000143-07-7	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	47





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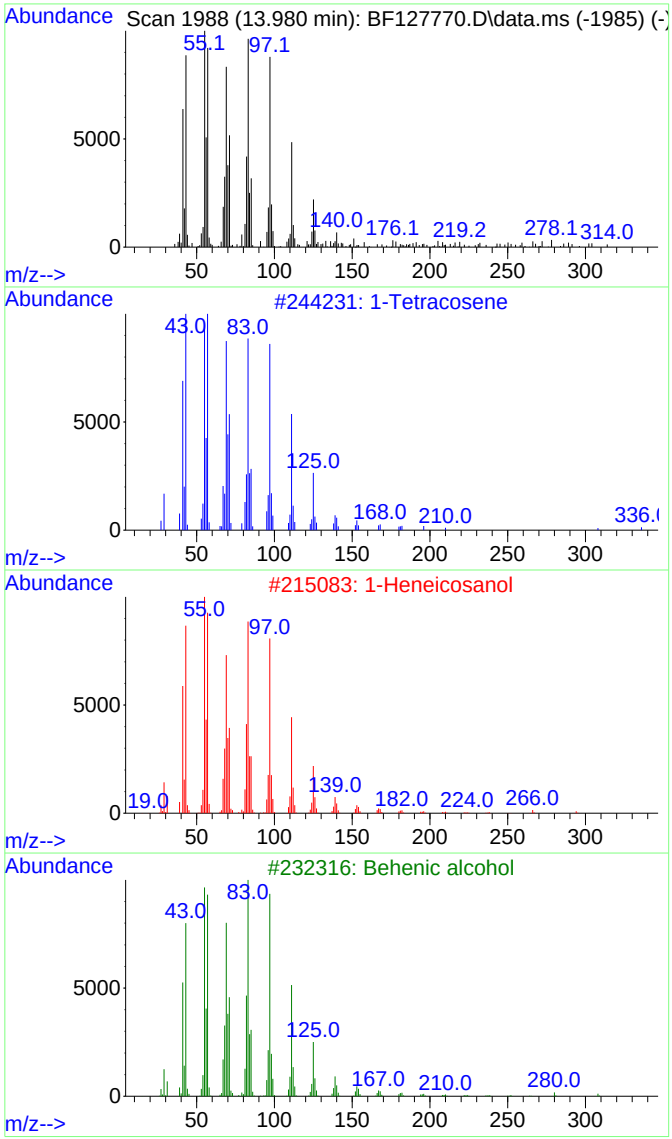
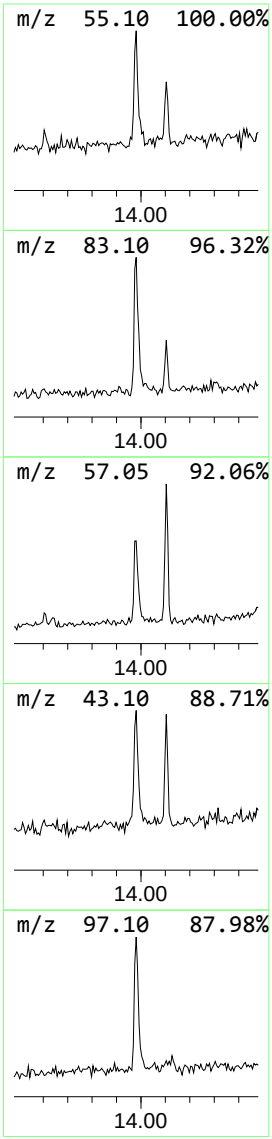
****

Peak Number 6 1-Tetracosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	4.62 ng	187975	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





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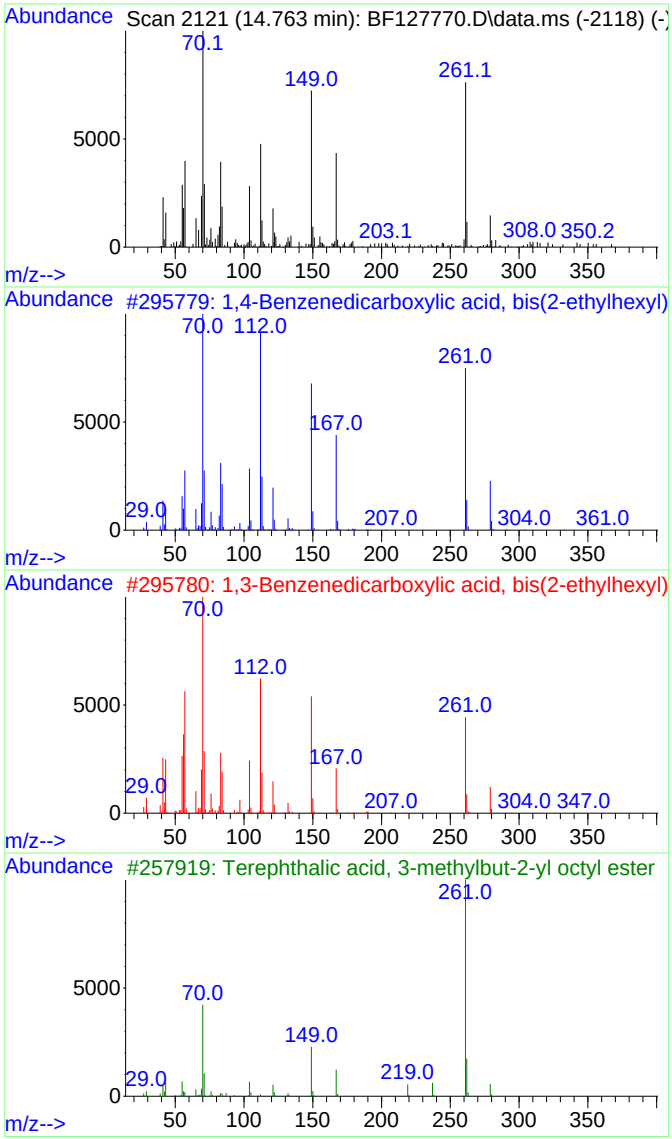
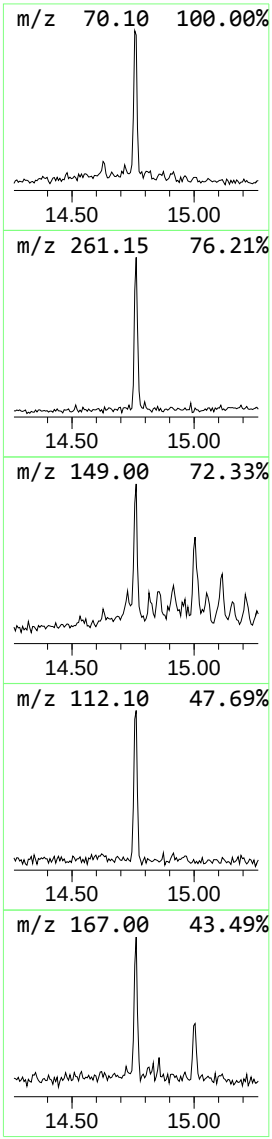
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	2.30 ng	93690	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
4	Terephthalic acid, 1-cyclopentyl...	374	C23H34O4	1010323-84-1	35
5	Isophthalic acid, 2-bromo-4-fluo...	450	C22H24BrFO4	1000344-40-1	27





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Furan, tetrahyd...	2.399	3.4	ng	129349	1	6.957	772906	20.0
unknown4.551	4.551	3.6	ng	140785	1	6.957	772906	20.0
unknown4.981	4.981	2.7	ng	105851	1	6.957	772906	20.0
2-Pentanone, 4-...	5.181	2.6	ng	100775	1	6.957	772906	20.0
n-Hexadecanoic ...	12.004	2.7	ng	130748	4	11.486	978392	20.0
1-Tetracosene	13.980	4.6	ng	187975	5	14.133	814430	20.0
1,4-Benzenedica...	14.763	2.3	ng	93690	5	14.133	814430	20.0