LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131786.D
Acq On : 22 Dec 2022 20:12
Operator : CG\JU
Sample : N6178-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131786.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	12	rVB	421443	514548	23.79%	3.028%
2	5.069	501	507	515	rVB	592921	763744	35.31%	4.495%
3	5.469	571	575	578	rBV	2045413	1820209	84.16%	10.712%
4	6.487	742	748	751	rBV	1832596	1853574	85.70%	10.909%
5	6.851	807	810	814	rVB	649271	501934	23.21%	2.954%
6	7.422	902	907	910	rBV	1352305	1215615	56.21%	7.154%
7	8.145	1025	1030	1033	rBV	661573	633575	29.29%	3.729%
8	9.222	1208	1213	1216	rBV	2431287	2162787	100.00%	12.729%
9	9.557	1267	1270	1273	rVB2	39830	31901	1.47%	0.188%
10	9.904	1325	1329	1332	rBV	962506	746365	34.51%	4.393%
11	10.451	1419	1422	1426	rVB	29093	23916	1.11%	0.141%
12	10.622	1447	1451	1455	rVB	38778	33105	1.53%	0.195%
13	10.698	1459	1464	1467	rBV	1728668	1502231	69.46%	8.841%
14	11.398	1579	1583	1585	rBV	917837	824366	38.12%	4.852%
15	11.422	1585	1587	1590	rVV	173099	136970	6.33%	0.806%
16	11.469	1590	1595	1598	rVB	61489	58858	2.72%	0.346%
17	11.922	1669	1672	1679	rVB2	139981	114363	5.29%	0.673%
18	12.010	1683	1687	1690	rBV2	26003	28371	1.31%	0.167%
19	12.610	1786	1789	1793	rVB	179058	148363	6.86%	0.873%
20	12.839	1823	1828	1834	rBV	125614	138037	6.38%	0.812%
21	12.986	1849	1853	1856	rBV	2341426	2110647	97.59%	12.422%
22	13.886	2003	2006	2024	rBV4	69824	230152	10.64%	1.355%
23	14.045	2026	2033	2036	rVV	672280	635284	29.37%	3.739%
24	14.068	2036	2037	2043	rVB	47423	33608	1.55%	0.198%
25	14.139	2044	2049	2056	rBV2	100506	110820	5.12%	0.652%
26	15.092	2207	2211	2215	rBV	27714	44356	2.05%	0.261%
27	15.163	2219	2223	2227	rVV2	22297	23898	1.10%	0.141%
28	15.468	2271	2275	2278	rBV	23322	27671	1.28%	0.163%
29	15.533	2281	2286	2299	rVB	352727	458290	21.19%	2.697%
30	15.998	2359	2365	2373	rBV2	38330	63901	2.95%	0.376%

Sum of corrected areas: 16991459

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131786.D
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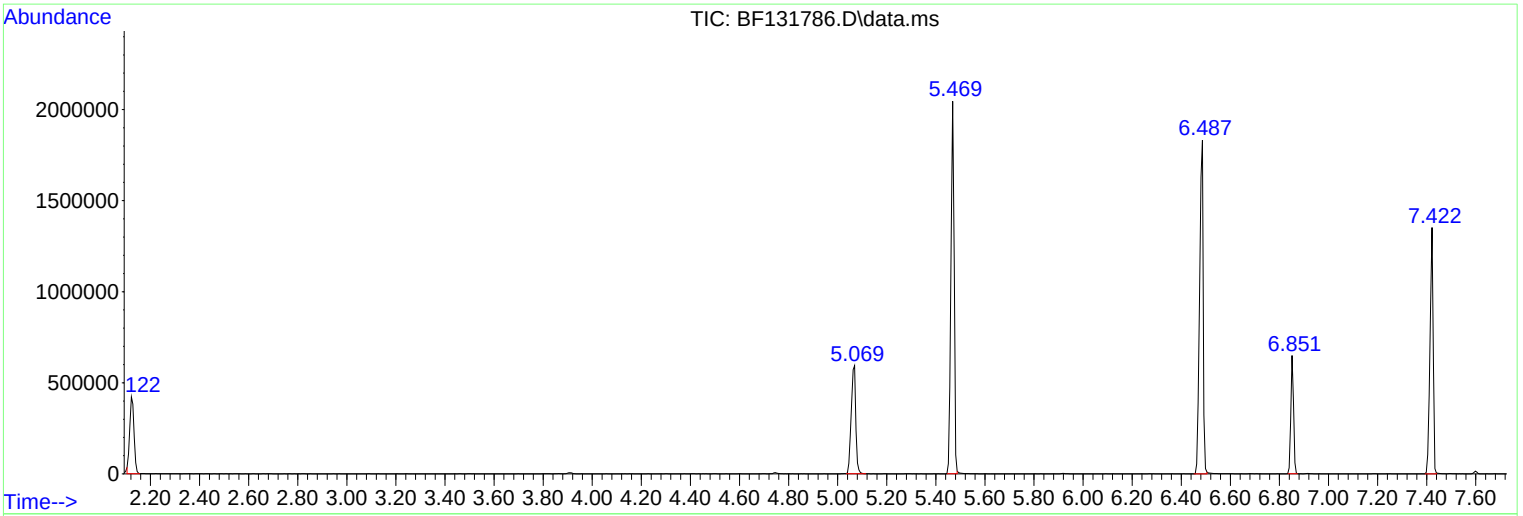
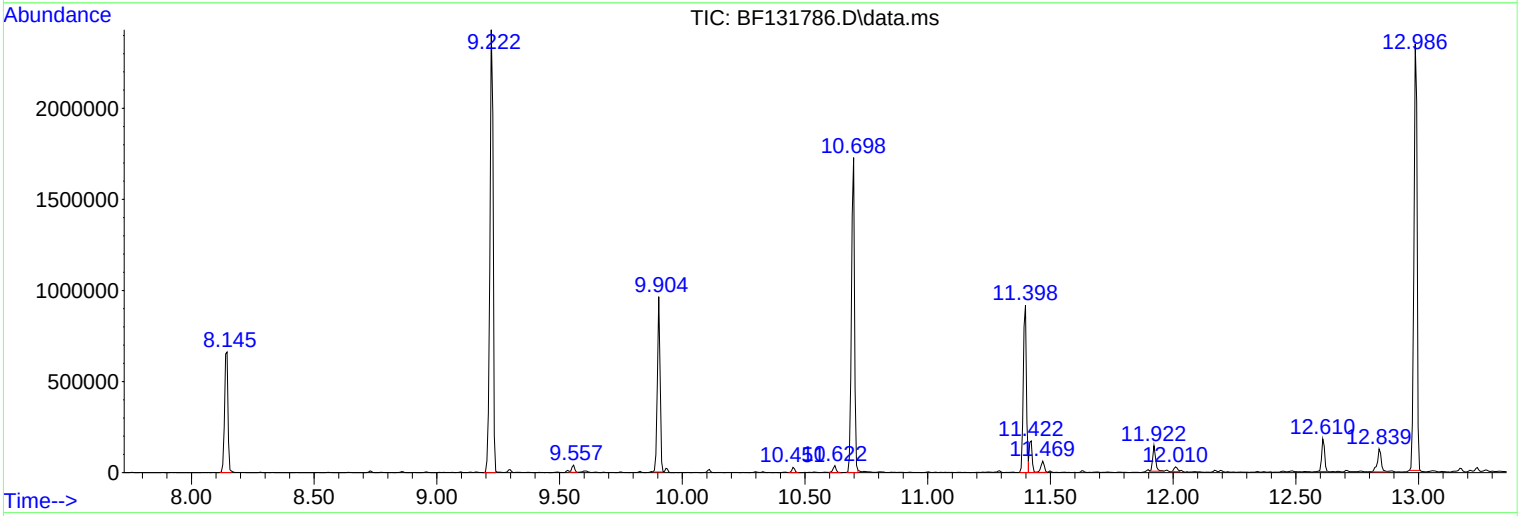
Operator : CG\JU
Sample : N6178-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

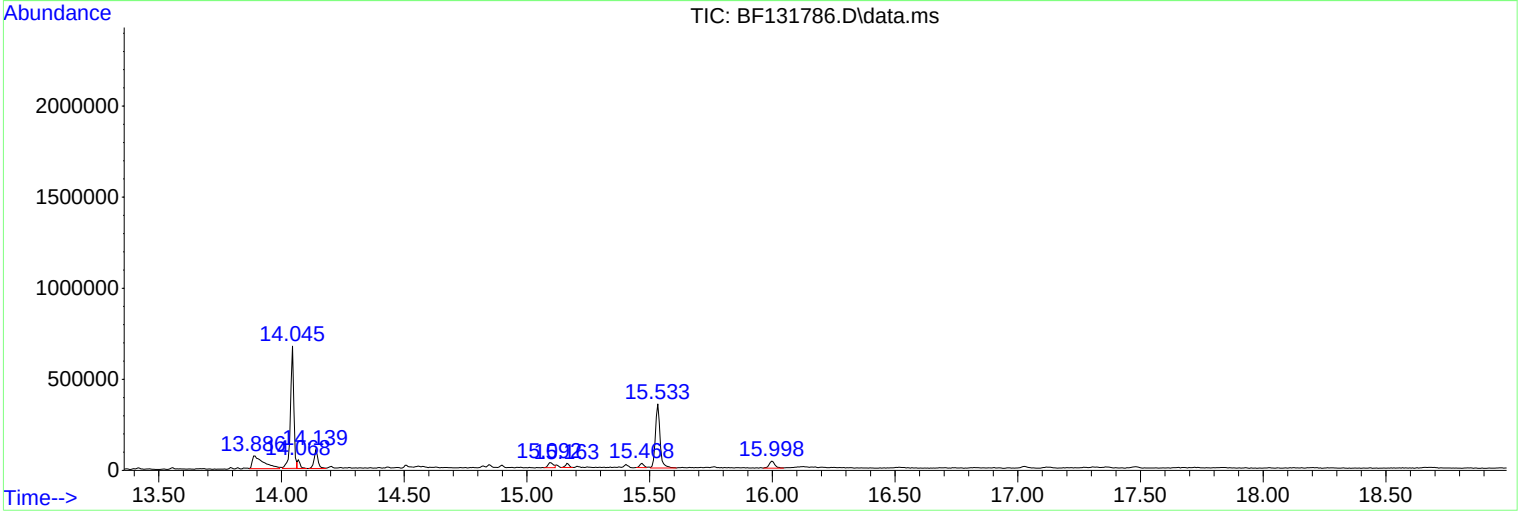
Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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\BF122222\
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

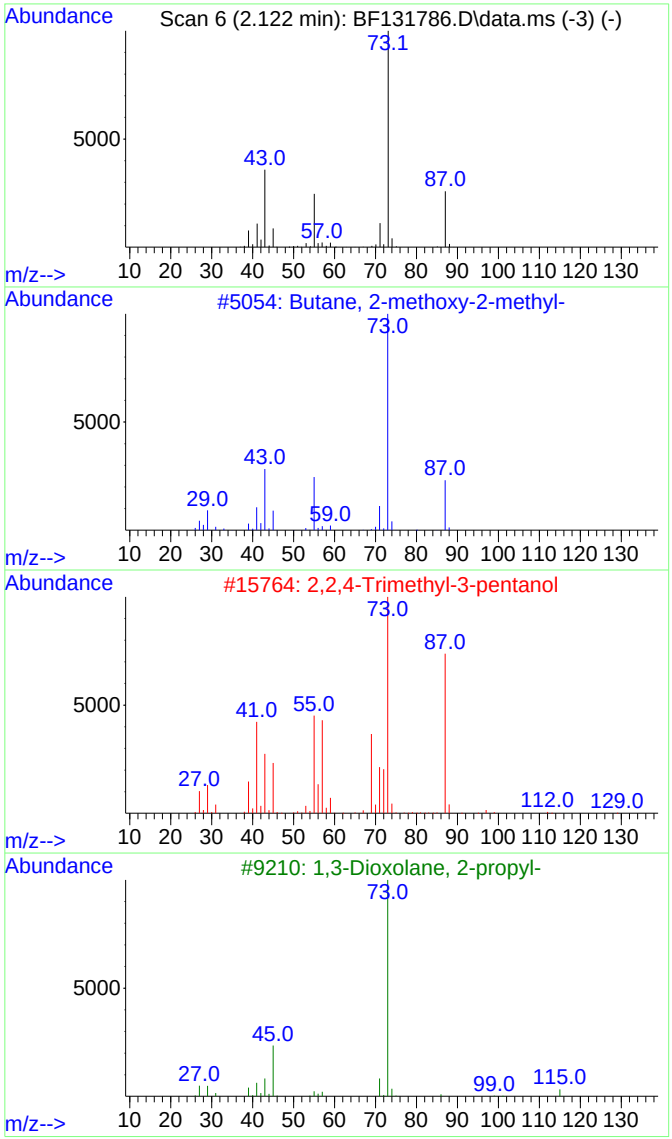
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

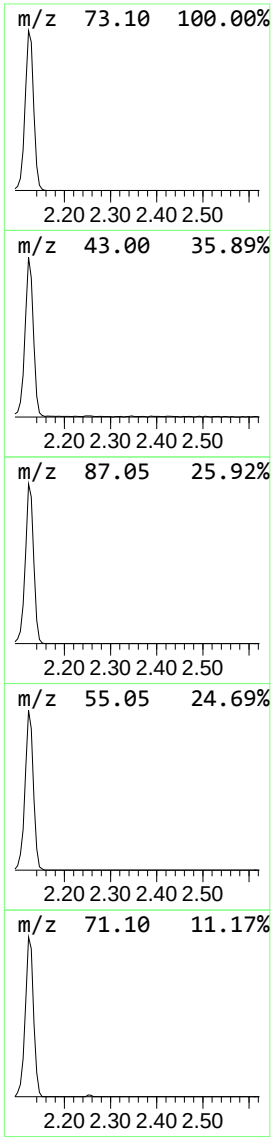
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	20.50 ng	514548	1,4-Dichlorobenzene-d4	6.851

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-propyl-	116	C6H12O2	003390-13-4	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Acq On : 22 Dec 2022 20:12
Operator : CG\JU
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Instrument :
BNA_F
ClientSampleId :
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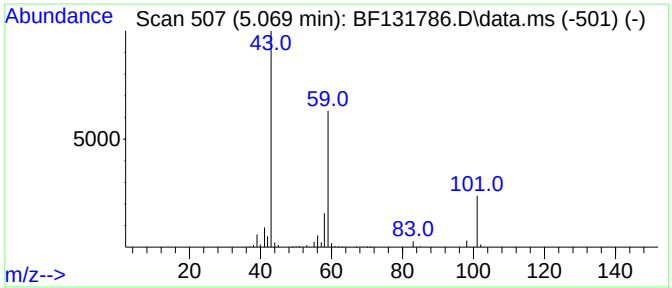
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

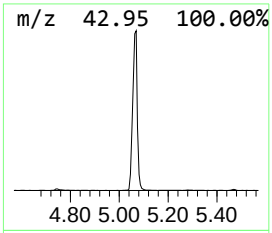
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

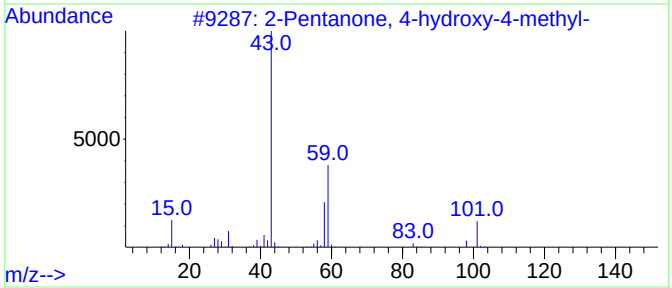
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

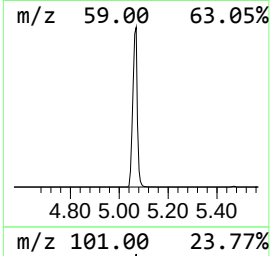
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	30.43 ng	763744	1,4-Dichlorobenzene-d4	6.851

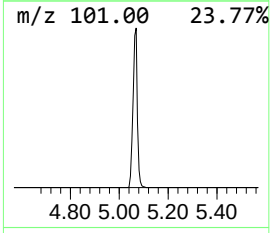
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

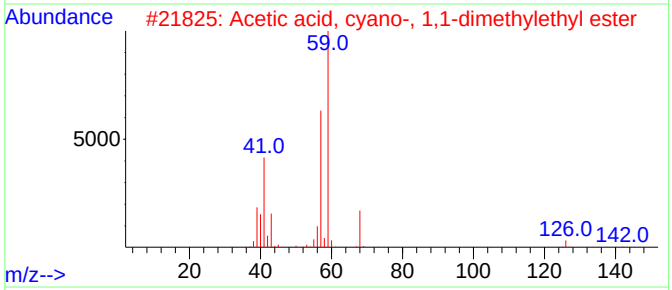


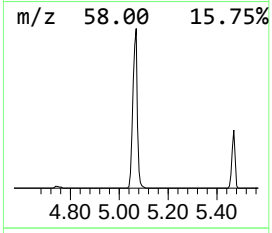


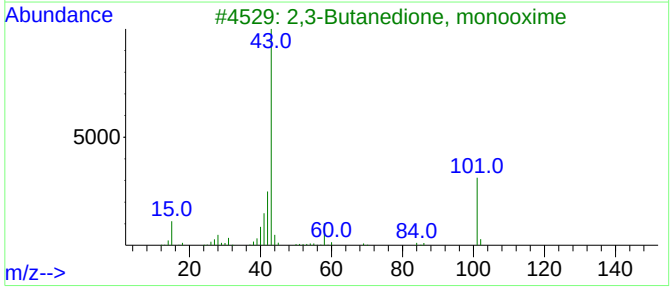


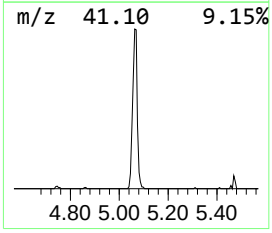












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Data File : BF131786.D
Acq On : 22 Dec 2022 20:12
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BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

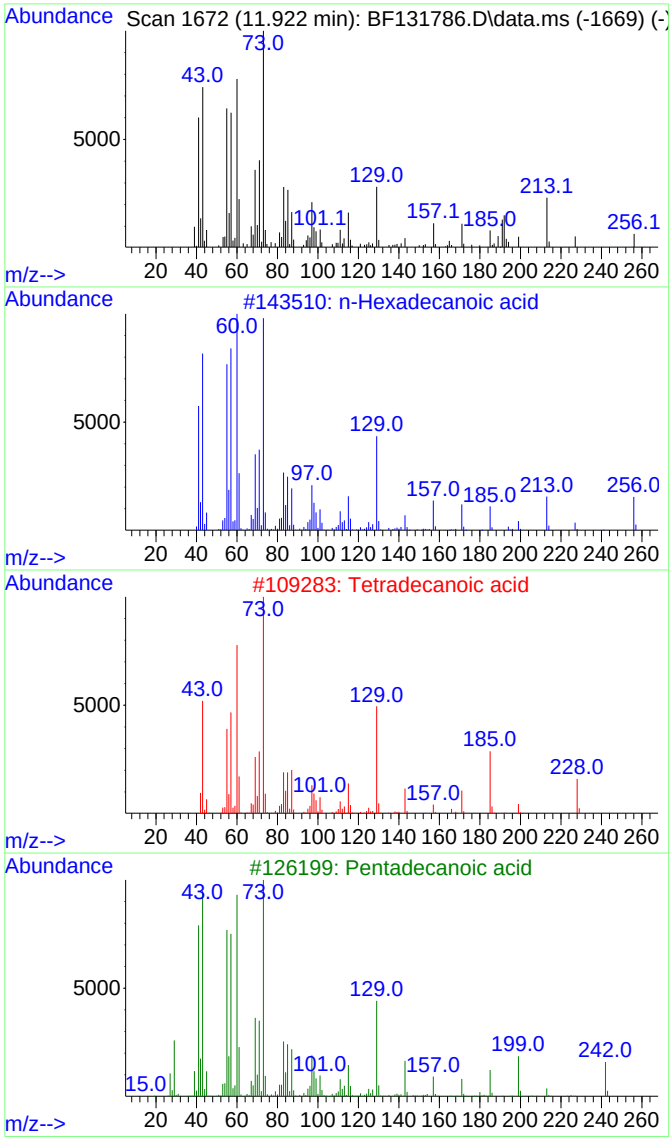
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

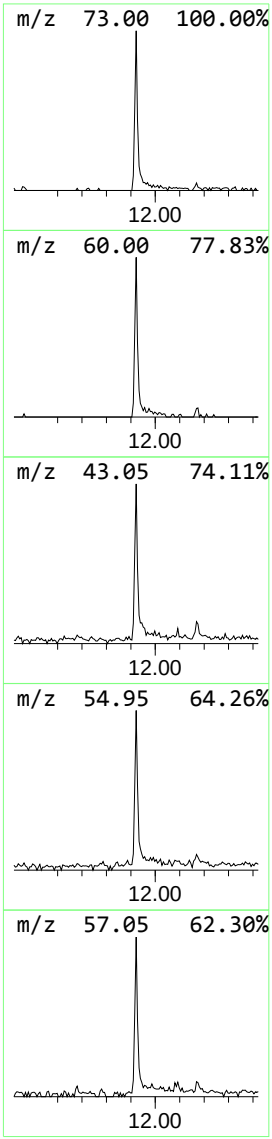
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.77 ng	114363	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	49
5	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

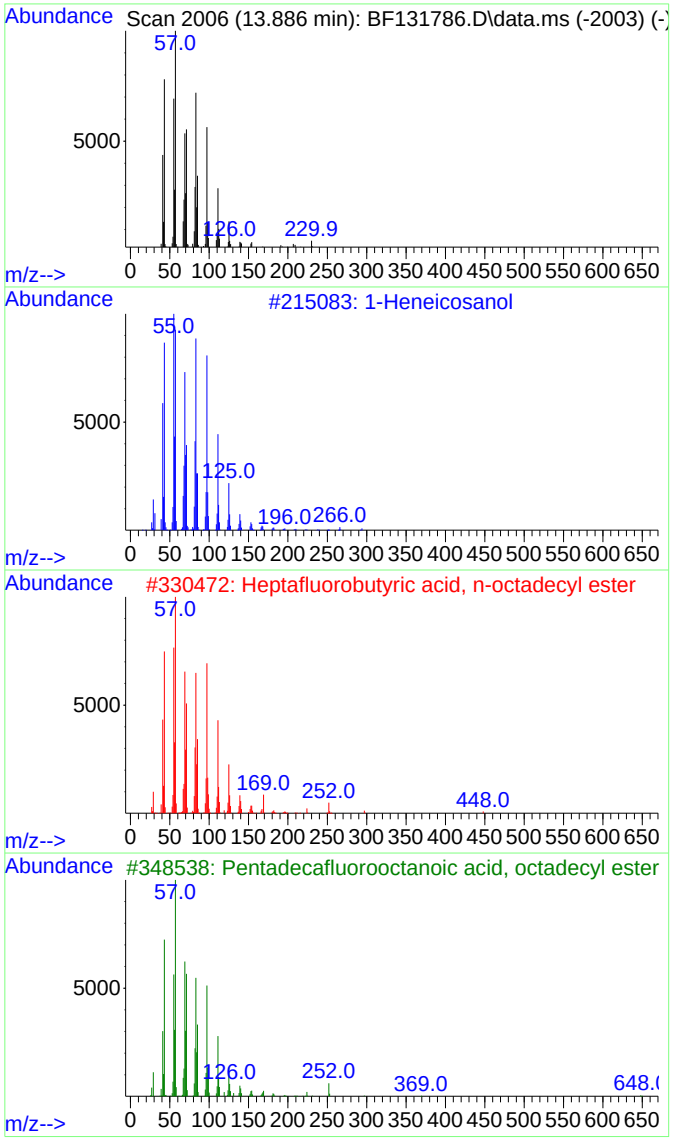
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

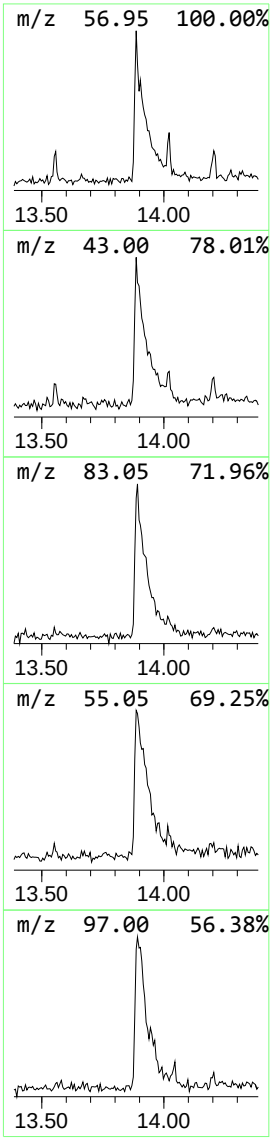
****

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	7.25 ng	230152	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91





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Data File : BF131786.D
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BNA_F
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COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

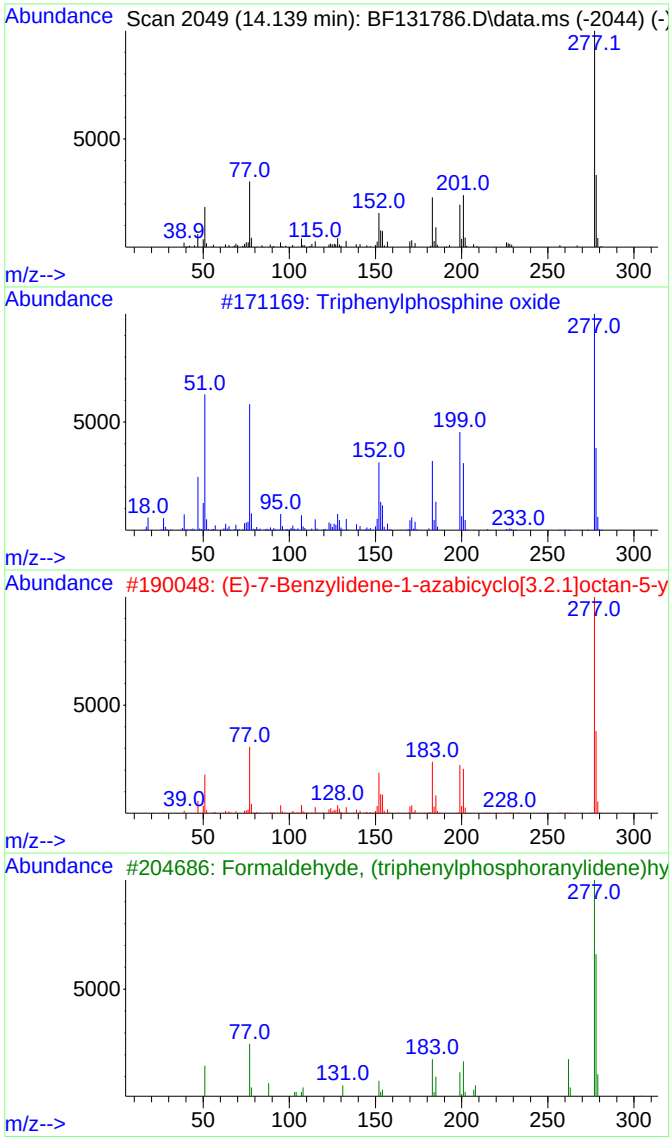
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

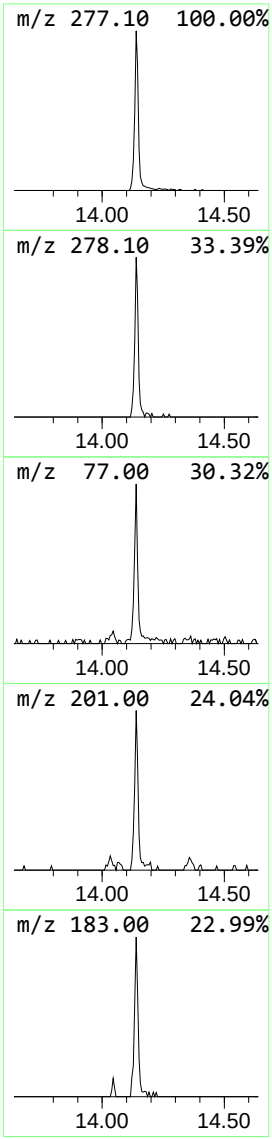
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	3.49 ng	110820	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38





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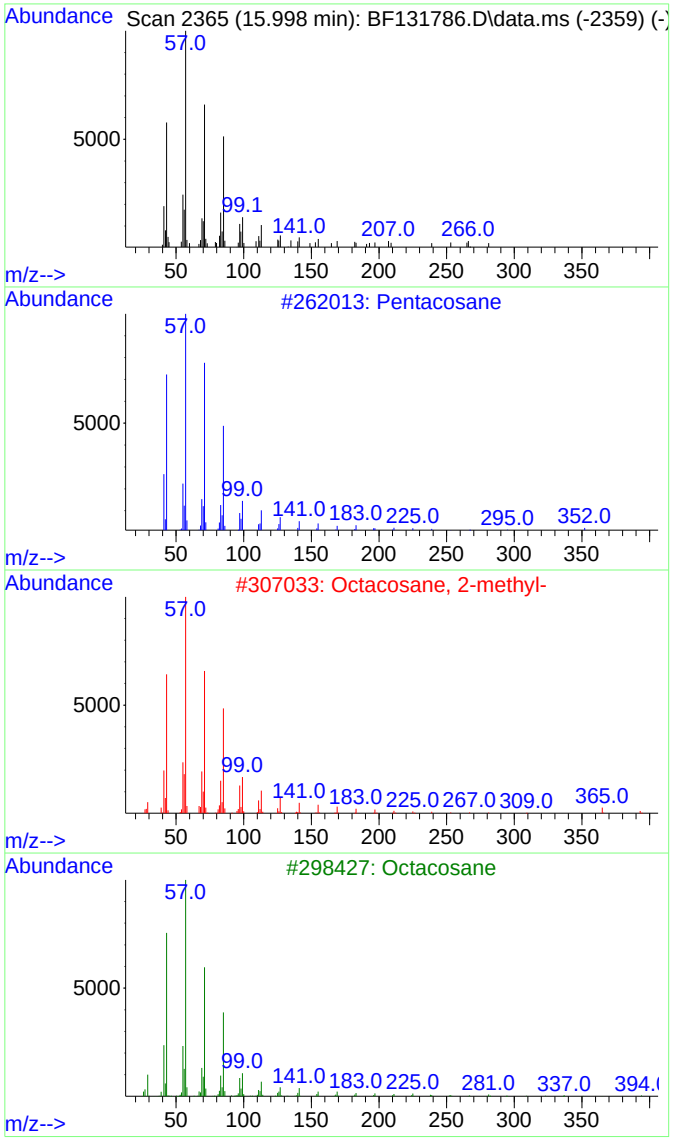
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

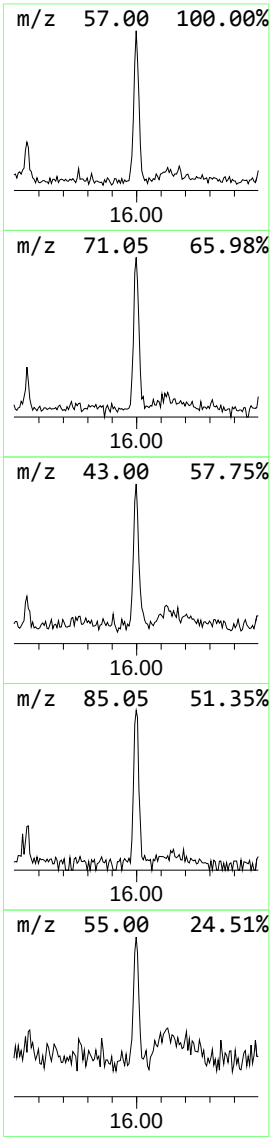
****

Peak Number 6 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.79 ng	63901	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Nonadecane	268	C19H40	000629-92-5	91





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-metho...	2.122	20.5	ng	514548	1	6.851	501934	20.0
2-Pentanone, 4-...	5.069	30.4	ng	763744	1	6.851	501934	20.0
n-Hexadecanoic ...	11.922	2.8	ng	114363	4	11.398	824366	20.0
1-Heneicosanol	13.886	7.3	ng	230152	5	14.045	635284	20.0
Triphenylphosph...	14.139	3.5	ng	110820	5	14.045	635284	20.0
Pentacosane	15.998	2.8	ng	63901	6	15.533	458290	20.0