LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081320\
Data File : BF121282.D
Acq On : 13 Aug 2020 21:10
Operator : JU/CG
Sample : L3508-13
Misc :
ALS Vial : 19 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TR-04-081220

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-BF081320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.240	361	366	372	rBV	34870	47633	2.15%	0.290%
2	4.892	473	477	486	rVB	870037	948850	42.76%	5.771%
3	5.322	546	550	565	rBV	816940	747439	33.69%	4.546%
4	6.357	722	726	738	rBV	1760953	1522787	68.63%	9.262%
5	6.722	784	788	791	rBV	681467	544552	24.54%	3.312%
6	7.286	880	884	887	rBV	1257537	1092296	49.23%	6.644%
7	8.004	1002	1006	1009	rBV	939296	720437	32.47%	4.382%
8	9.080	1185	1189	1192	rBV	2502616	2080147	93.75%	12.652%
9	9.474	1252	1256	1260	rBV	164862	139306	6.28%	0.847%
10	9.751	1300	1303	1307	rVB	945485	829163	37.37%	5.043%
11	10.663	1455	1458	1466	rBV4	22367	36067	1.63%	0.219%
12	11.233	1551	1555	1558	rBV	1034944	889654	40.10%	5.411%
13	11.633	1620	1623	1626	rBV	61986	69112	3.11%	0.420%
14	12.033	1688	1691	1693	rBV2	79199	97345	4.39%	0.592%
15	12.315	1737	1739	1741	rBV	109475	110768	4.99%	0.674%
16	12.821	1820	1825	1828	rBV	2405574	2218852	100.00%	13.495%
17	13.068	1863	1867	1869	rBV4	39202	67690	3.05%	0.412%
18	13.739	1976	1981	1988	rBV4	153688	428720	19.32%	2.608%
19	13.868	1999	2003	2006	rVB	851706	749729	33.79%	4.560%
20	14.721	2144	2148	2162	rVB2	464363	1431135	64.50%	8.704%
21	15.286	2240	2244	2248	rBV	552045	640042	28.85%	3.893%
22	16.374	2419	2429	2443	rVB4	233935	1029829	46.41%	6.264%

Sum of corrected areas: 16441553

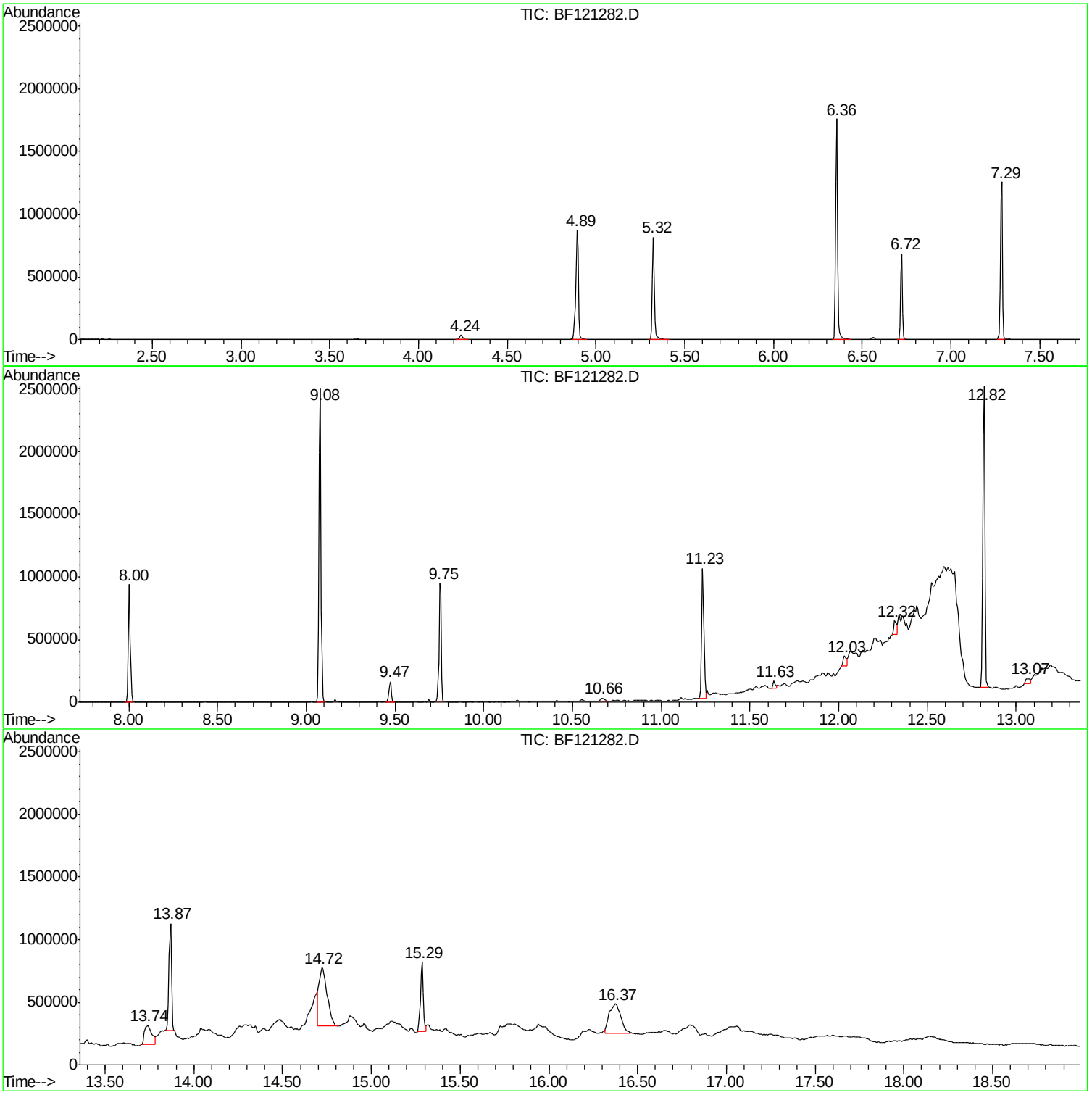
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081320\
Data File : BF121282.D
Acq On : 13 Aug 2020 21:10
Operator : JU/CG
Sample : L3508-13
Misc :
ALS Vial : 19 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
TR-04-081220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081320\
Data File : BF121282.D
Acq On : 13 Aug 2020 21:10
Operator : JU/CG
Sample : L3508-13
Misc :
ALS Vial : 19 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TR-04-081220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

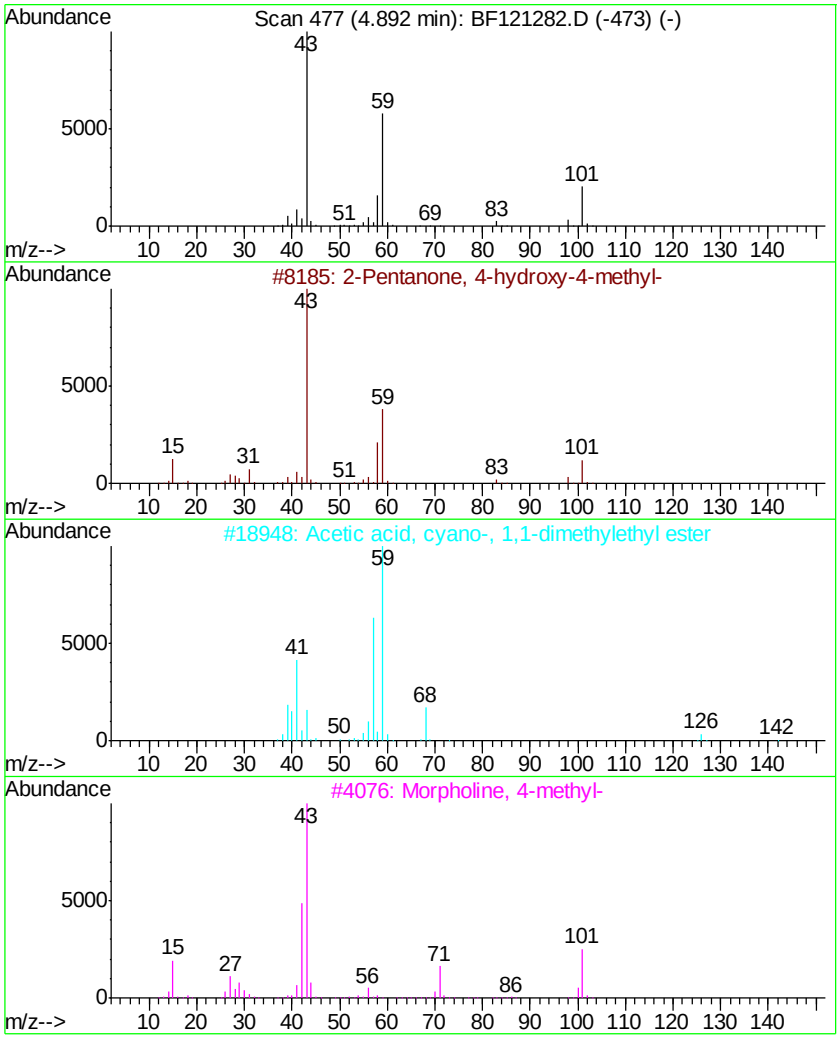
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

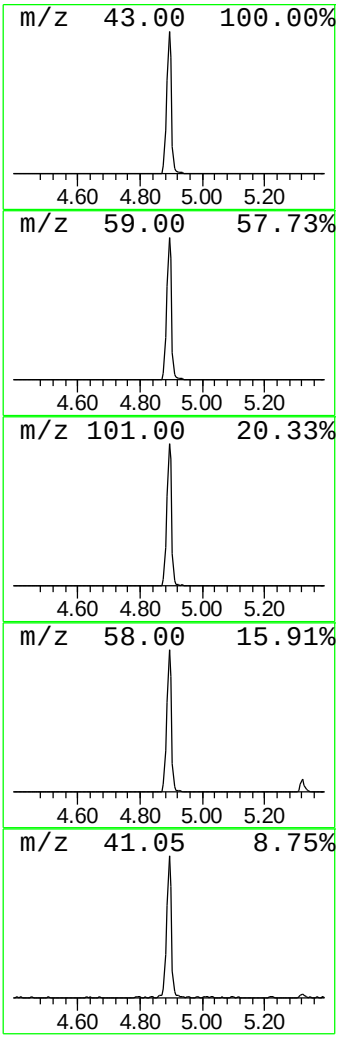
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	34.85 ng	948850	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081320\
Data File : BF121282.D
Acq On : 13 Aug 2020 21:10
Operator : JU/CG
Sample : L3508-13
Misc :
ALS Vial : 19 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TR-04-081220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

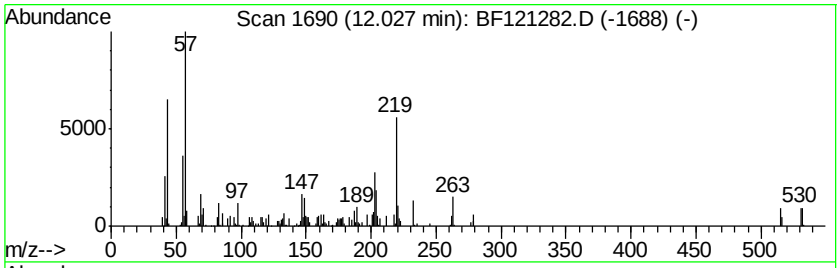
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

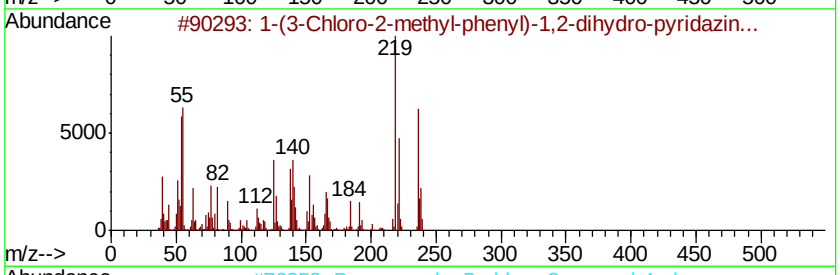
****

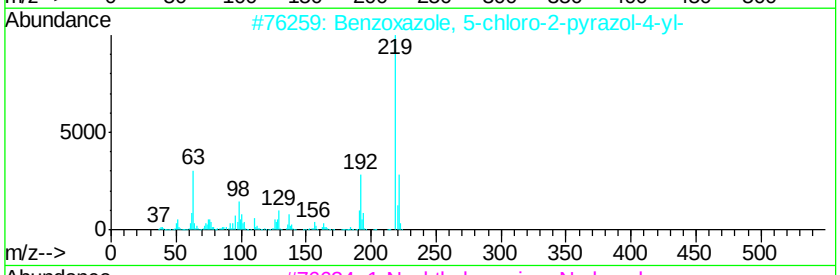
Peak Number 2 unknown12.03 Concentration Rank 6

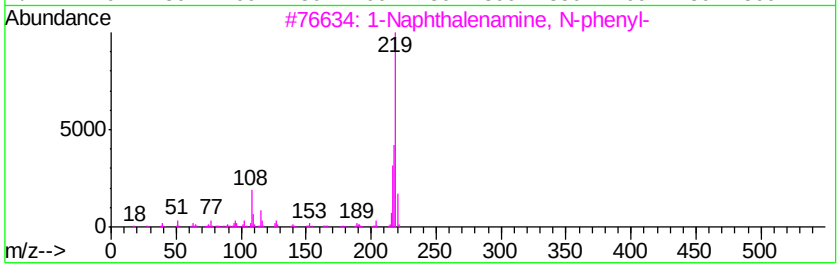
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	2.19 ng	97345	Phenanthrene-d10	11.23

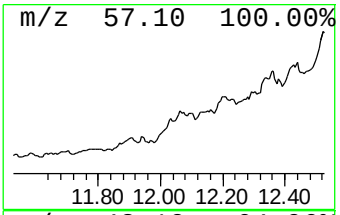
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Chloro-2-methyl-phenyl)-1,2...	236	C11H9ClN2O2	1000294-43-8	46
2	Benzoxazole, 5-chloro-2-pyrazol-...	219	C10H6ClN3O	1000262-42-6	43
3	1-Naphthalenamine, N-phenyl-	219	C16H13N	000090-30-2	43
4	Hydrido-iron(II), (.eta.-5-penta...	386	C19H40FeP2	1000162-78-8	38
5	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	38

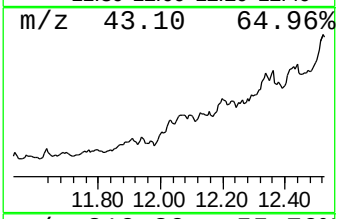


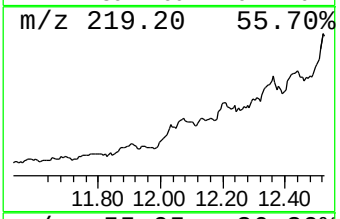


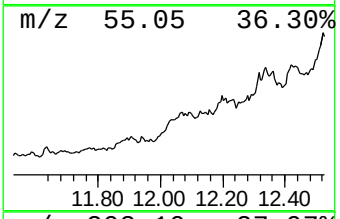


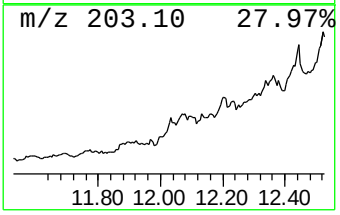












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Data File : BF121282.D
Acq On : 13 Aug 2020 21:10
Operator : JU/CG
Sample : L3508-13
Misc :
ALS Vial : 19 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TR-04-081220

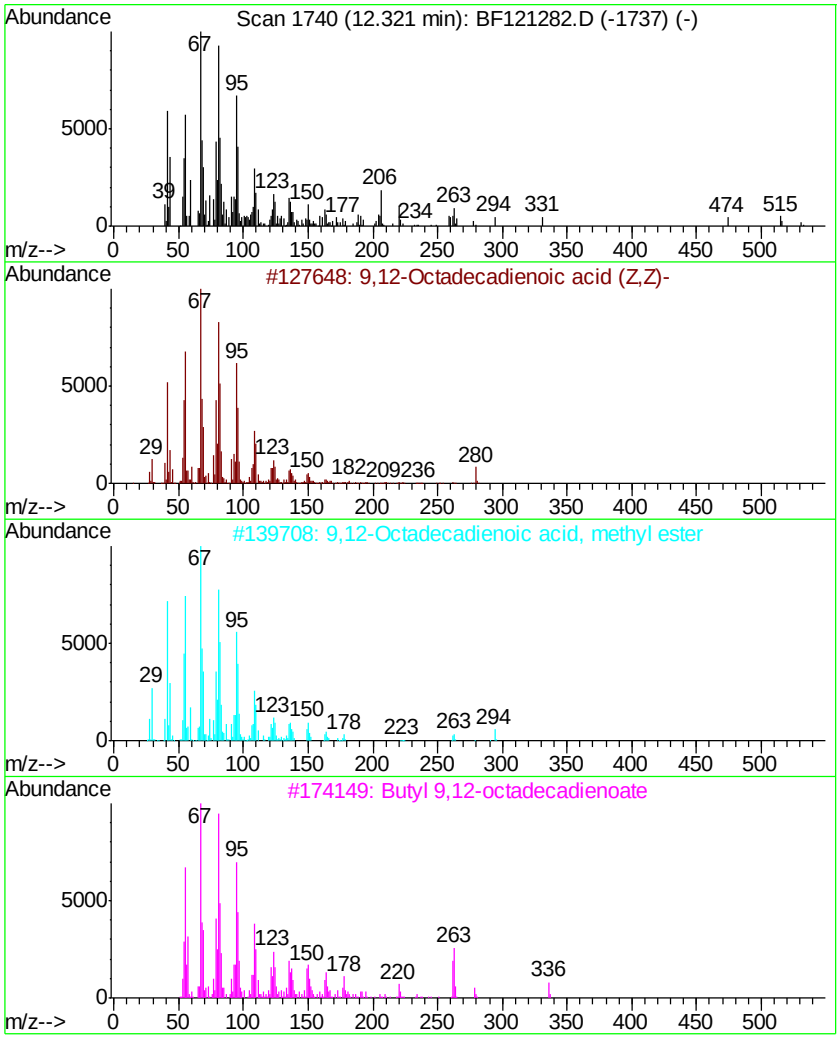
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

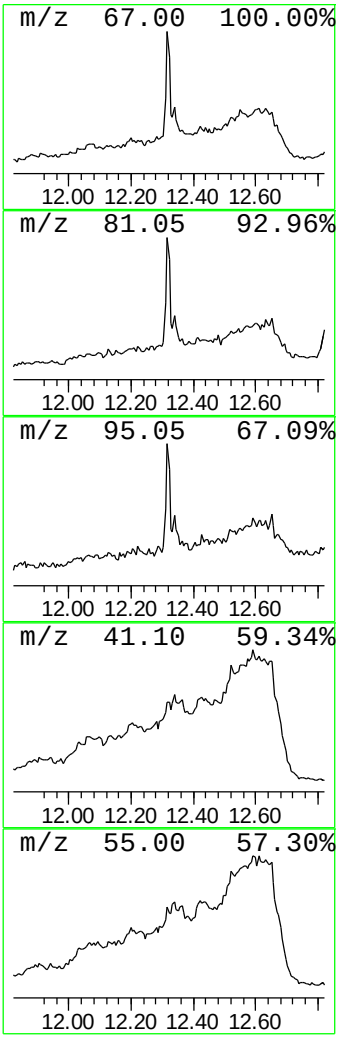
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	2.49 ng	110768	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	87
3	Butyl 9,12-octadecadienoate	336	C22H40O2	1000336-54-1	87
4	n-Propyl 9,12-octadecadienoate	322	C21H38O2	1000336-77-8	87
5	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	83





Library Search Compound Report

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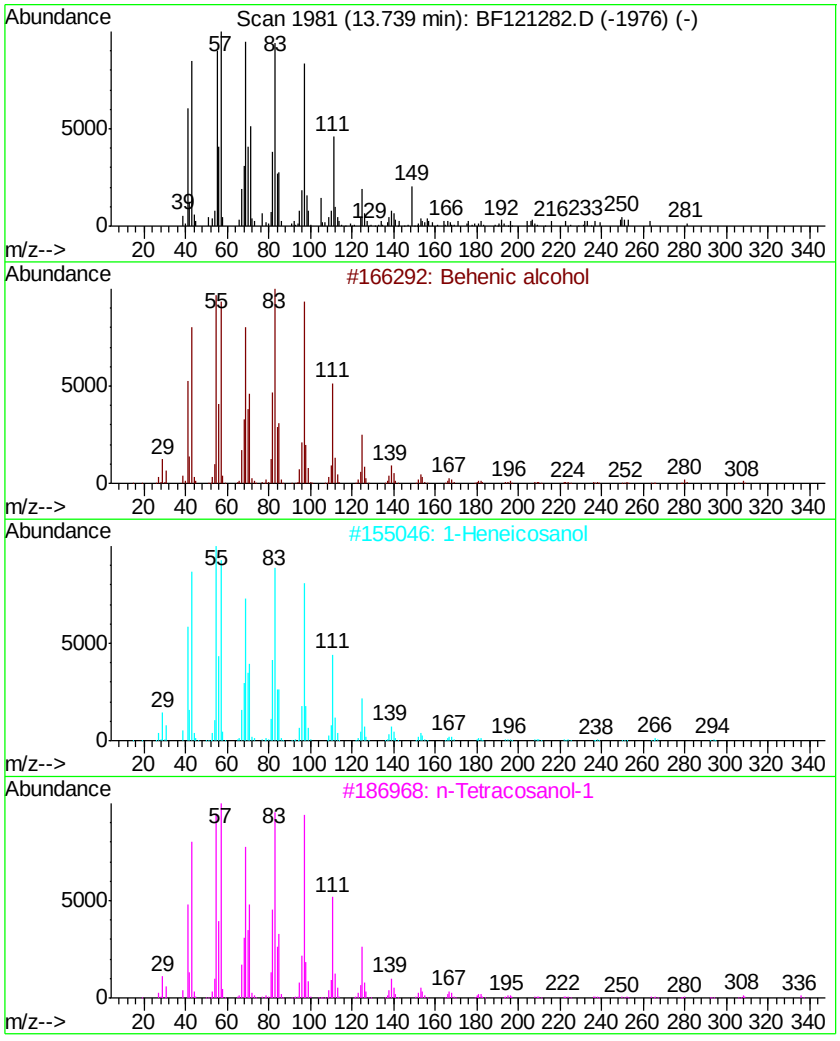
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

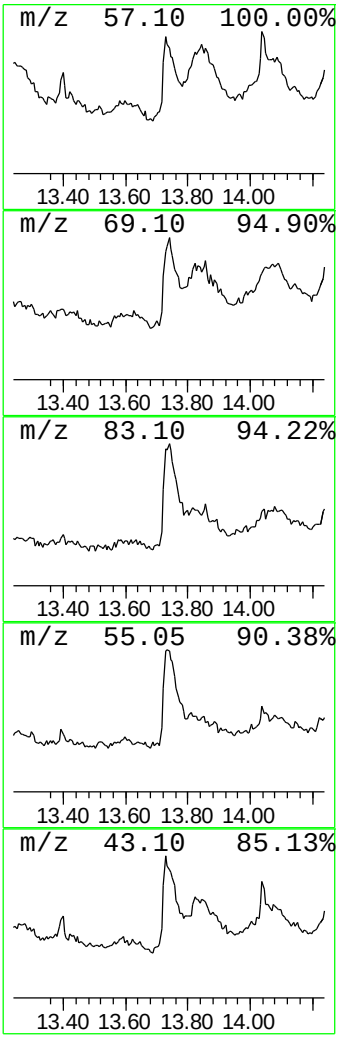
****

Peak Number 4 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	11.44 ng	428720	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	92
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	89





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Misc :
ALS Vial : 19 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TR-04-081220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

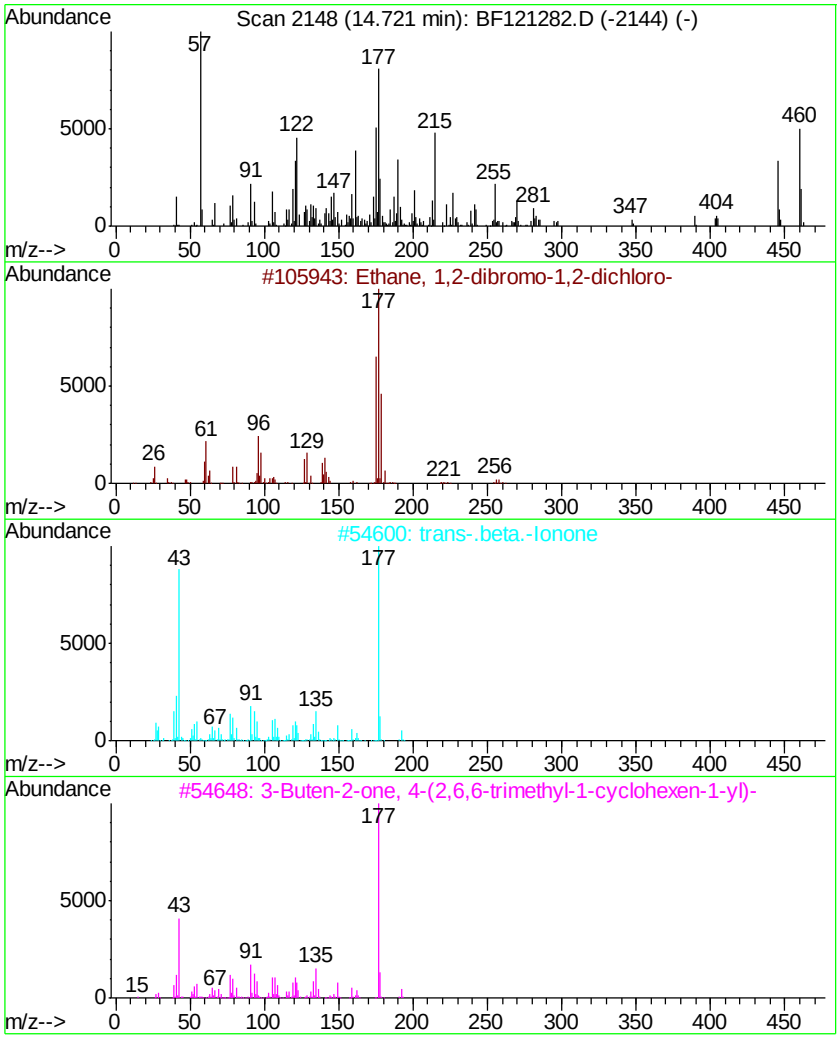
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

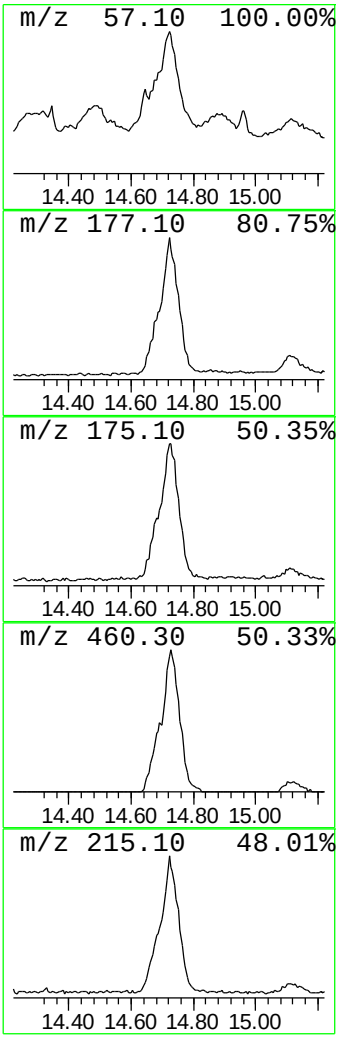
****

Peak Number 5 unknown14.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	44.72 ng	1431140	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,2-dibromo-1,2-dichloro-	254	C2H2Br2Cl2	000683-68-1	22
2	trans-.beta.-Ionone	192	C13H20O	000079-77-6	11
3	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	11
4	4(1H)-Pteridinone, 2-amino-6-met...	177	C7H7N5O	000708-75-8	10
5	5-Aminomethylene-6-hydroxy-4-met...	177	C8H7N3O2	1000223-27-4	10





Library Search Compound Report

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ClientSampleId : TR-04-081220

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

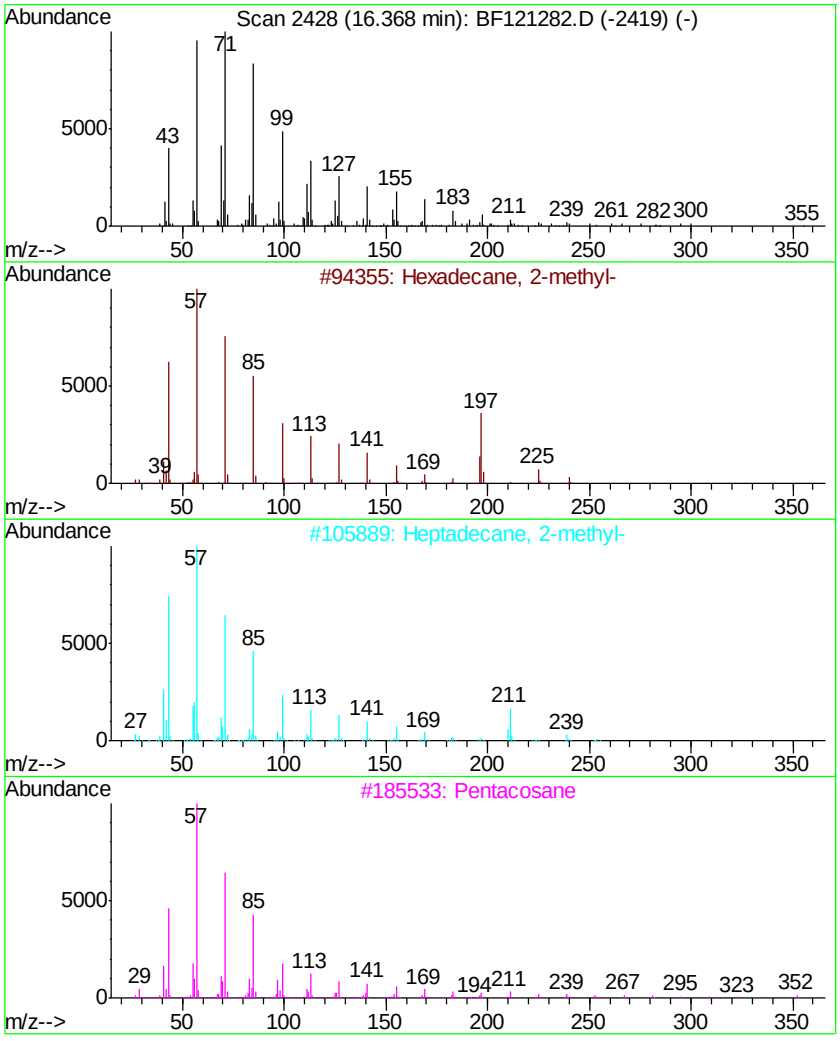
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

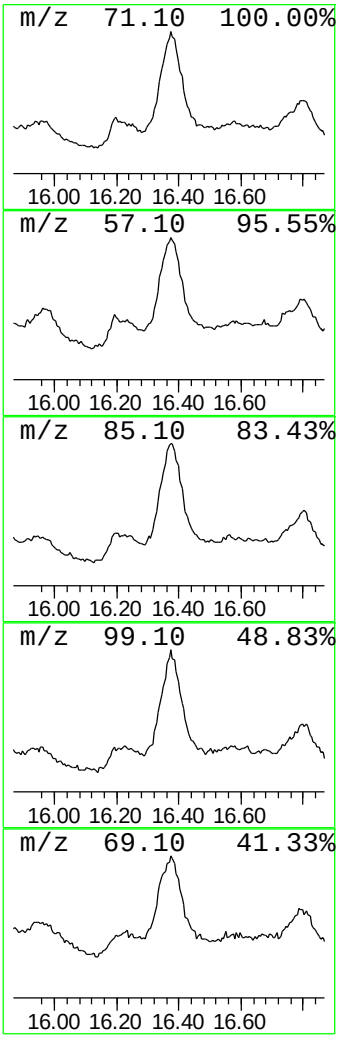
****

Peak Number 6 Hexadecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	32.18 ng	1029830	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	80
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	78
3	Pentacosane	352	C25H52	000629-99-2	78
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	58





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	34.9	ng	948850	1	6.72	544552	20.0
unknown12.03	12.03	2.2	ng	97345	4	11.23	889654	20.0
9,12-Octadecadien...	12.32	2.5	ng	110768	4	11.23	889654	20.0
Behenic alcohol	13.74	11.4	ng	428720	5	13.87	749729	20.0
unknown14.72	14.72	44.7	ng	1431140	6	15.29	640042	20.0
Hexadecane, 2-met...	16.37	32.2	ng	1029830	6	15.29	640042	20.0